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User's Guide for Executing OZIPM-4 (Ozone Isopleth Plotting with Optional Mechanisms Version 4) with CBM-IV (Carbon-Bond Mechanism-IV) or Optional Mechanisms. Volume 1

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An updated version of the Ozone Isopleth Plotting Program has been developed for use with EKMA to calculate emission reductions needed to achieve the air quality standard for ozone. The program, called OZIPM-IV (Ozone Isopleth Plotting with Optional Mechanisms - Version IV), contains the new Carbon-Bond Mechanism-IV (CBM-IV). In addition to containing a new mechanism, the OZIPM-IV expands on earlier versions of the code by providing a wider compatibility between computers, an improved isopleth plotting package, expanded user interaction with control strategy calculations and a new option for determining credits for reductions in carbon monoxide emissions. Volume 1 of the report serves as the User's Manual for OZIPM-IV. Volume 2 contains the listing of the FORTRAN computer code.

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Volume 1

Description of the Ozone Isopleth Plotting Package Version 4

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ABSTRACT

The U.S. Environmental Protection Agency is continuing to recommend the use of the Empirical Kinetic Modeling Approach (EKMA) as a procedure for relating levels of photochemical ozone to levels of volatile organic compounds and oxides of nitrogen. In a recent study Systems Applications developed a new chemical mechanism called the Carbon-Bond Mechanism-IV (CBM-IV), which provides a complete and verified description of urban smog chemistry. In this study, the CBM-IV has been incorporated into a new computer program called Ozone Isopleth Plotting with Optional Mechanisms--Version 4 (OZIPM-4). This program is designed to be used with EKMA to calculate the emission reductions needed to achieve the air quality standard for ozone. The OZIPM-4 program can accept as input chemical mechanisms other than the CBM-IV. Recent updates and improvements to the OZIPM-4 program are discussed herein, along with the CBM-IV mechanism. OZIPM-4 expands on earlier codes by providing a wider compatibility between computers, an improved isopleth plotting package, expanded user interaction with control strategy calculations, and a new option for determining credits for carbon monoxide emissions reductions. Volume 1 of this report serves as the User's Manual for OZIPM-4. It contains both a detailed description of OZIPM-4 and a discussion of the input and output requirements and options available for exercising either the default CBM-IV mechanism or an optional mechanism. Five examples of OZIPM-4 input and output files are also included. Volume 2 contains the listing of the FORTRAN computer code. A magnetic tape or floppy disk of this code is also available from Systems Applications.

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SECTION 1

OVERVIEW

BACKGROUND AND PURPOSE

The U.S. Environmental Protection Agency (EPA) recommends two approaches for formulating State Implementation Plans (SIP) for attainment of the ozone National Ambient Air Quality Standard (NAAQS). One of these is the city-specific Empirical Kinetic Modeling Approach (EKMA), which is described in a guideline document issued in March 1981 (EPA, 1981). The other approach refers to the use of large, sophisticated air quality simulation models (AQSMs) such as the Systems Applications Urban Airshed Model.

EKMA was developed as a procedure for relating levels of photochemical oxidants (expressed as ozone) to levels of nonmethane organic compounds (NMOC) and oxides of nitrogen (NO_x) (EPA, 1977); it utilizes a set of isopleths that depict maximum afternoon concentrations of ozone as a function of the following parameters:

Morning concentrations of NMOC and NO_x (which may include precursors transported from upwind sources);

Emissions of volatile organic compounds (VOC), NO_x, and other species (such as carbon monoxide) occurring during the day;

Meteorological conditions; and

Reactivity of different VOC and NMOC mixtures.

The isopleths are developed through multiple computer simulations using different levels of NMOC and NO_x concentrations. The calculated maximum hourly ozone concentrations are then used to generate ozone concentration isolines that are plotted as a function of initial precursor concentrations. These isopleths are used to compute the percent reduction in emissions that is needed to lower peak ozone to the NAAQS of 0.12 ppm.

A computer program was developed to readily generate the ozone isopleth for EKMA users. This program, which is called the Ozone Isopleth Plotting Package (OZIPP), has been documented by Whitten and Hogo (1978a). Since its formulation, more sophisticated versions of the OZIPP have been developed:

> OZIPM--Version 1--a computer routine with the capability of accepting different chemical kinetics mechanisms as input (Whitten and Hogo, 1978b).
>
> OZIPM--Version 2--this version of OZIPM contains some code modifications to the original version so that it can be used easily on different computer systems; it also has the capability of calculating the needed percent reduction in VOC without first generating an isopleth (Gipson, 1984).
>
> OZIPM--Version 3--a newer mechanism, called the CBM-X, was incorporated into this version. The results of that work are described in Hogo and Whitten (1985) and Whitten et al. (1985).
>
> OZIPM--Version 4--the current version--is an update to OZIPM-3. This version requires less computer memory and some program modifications have been made to correct computer errors associated with OZIPM-3. In addition, a new mechanism called CBM-IV (Gery, Whitten, and Killus, 1988) has been coded into this version. OZIPM-4 also contains a new option for specifically determining future-year ozone levels resulting from changes in carbon monoxide emissions.

The purpose of this two-volume report is to provide guidelines for using OZIPM-4 with the CBM-IV (or other mechanisms). This volume serves as the User's Manual for OZIPM-4. Section 2 of this volume contains an overall technical description. Section 3 presents a detailed description of the different input and output options available with the OZIPM-4. Section 4 provides guidance on the selection of input options when using the CBM-IV stored in OZIPM-4. Section 5 contains a summary of the options discussed in Sections 3 and 4, and serves as a quick reference guide for the user. Section 6 contains examples of model runs that demonstrate the use and flexibility of OZIPM-4. Volume 2 contains the computer code listing for OZIPM-4. A magnetic tape of this program can be purchased from the National Technical Information Service, Springfield, Virginia 22161, telephone (703) 557-4650, or from Systems Applications, Inc., 101 Lucas Valley Road, San Rafael, California 94903, telephone (415) 472-4011.

LIMITATIONS

OZIPM-4 has a limited applicability to ozone problems within, or immediately downwind of, large urban areas and thus should not be applied to the following situations unless special attention is given to current limitations and assumptions:

The rural ozone problem;

Situations in which transported ozone and/or precursors are clearly dominant (i.e., multiday transport situations);

Cases in which the maximum ozone concentration occurs at night or in the early morning; and

The development of control strategies for single or small groups of emission sources.

The validity of an ozone isopleth diagram generated by OZIPM-4 for a particular city may be limited by the following considerations:

The kinetic mechanism used to describe the transformations of NMOC and NO_x;

The physical assumptions used to formulate the trajectory model coded into OZIPM-4;

The meteorological data and assumptions used to specify required OZIPM-4 parameters;

The availability and reliability of current ozone data, precursor concentration data, and VOC, NO_x, and CO emission inventories;

The mathematical assumptions needed to integrate the differential equations formulated within OZIPM-4; and

The interpolations needed to generate isopleths from the results of a number of computer simulations.

Because these considerations are part of the basic definitions and concepts that constitute OZIPM-4 and EKMA, they are explained more fully in the following sections.

BASIC DEFINITIONS

Kinetic Mechanism

A kinetic mechanism is a set of chemical reactions and rate constants that describes some chemical process. Using a kinetic mechanism, one can derive coupled, first-order, nonlinear, ordinary differential equations that describe the rates of change of pollutant concentrations with time. These equations can then be integrated with a computer to simulate the changing pollutant concentrations in a smog chamber or in the atmosphere.

The original version of this program (OZIPP) used a two-hydrocarbon/NO_x mechanism to describe the photochemical formation of ozone (Dodge, 1977). In that mechanism, propylene and butane are used as surrogates to represent the urban mix of emissions. The propylene-to-butane ratio of 1:3 in that mechanism cannot be adjusted to account for the changing reactivity of the urban hydrocarbon mix. Because of this and other shortcomings of the original OZIPP program, many users indicated the need for a more flexible chemical mechanism. The Carbon-Bond Mechanism-III (CBM-III) (Killus and Whitten, 1984) was one such mechanism. An expanded version of the CBM-III known as the extended Carbon-Bond Mechanism (CBM-X) was later incorporated in OZIPM-3 as the default chemical mechanism. Now, a new condensed mechanism, the CBM-IV (Gery, Whitten, and Killus, 1988), has been included in the OZIPM-4.

Use of the CBM-IV in OZIPM-4 provides the following advantages:

(1) The CBM-IV is more responsive to a wider range of reactivity than earlier mechanisms.

(2) Reactivity is more clearly defined as a function of more and better resolved reactivity groups.

(3) The CBM-IV is based on the most recent kinetic and product data available at the time of its development.

(4) The CBM-IV has been validated with more extensive smog chamber data than that used to validate earlier mechanisms.

Precursors of Ozone

Precursors of ozone are the chemical species that react to form ozone. The primary precursors are total organic compounds (TOC) and oxides of nitrogen (NO_x). The EPA guidelines (EPA, 1981) on the use of city-specific EKMA contain two definitions of organic compounds. The first definition, termed "VOC" or volatile organic compounds, represents the sum of the reactive organic emissions included in emission inventories. The second definition, termed "NMOC" or nonmethane organic compounds, represents ambient measurements of all organic compounds other than methane. Both VOC and NMOC are organic precursors of ozone. Methane is not considered a precursor because it reacts very slowly. In this document, organic compounds associated with emission inventories will be termed "VOC". Organic compounds associated with the background and initial concentrations in the surface and aloft layers will be termed "NMOC" because these are typically associated with ambient measurements rather than with emission inventories. NO_x, as used in this report, signifies the sum of the concentrations of nitric oxide (NO) and nitrogen dioxide (NO_2).

Simulation

A computer simulation involves the calculation of the concentrations of pollutants found in the kinetic mechanism as a function of time. Concentrations are reported at various times specified by the user. The calculations involve the integration of a set of coupled, first-order, nonlinear, ordinary differential equations defined by the kinetic mechanisms that describe the chemical and physical processes underlying the model. User-specified assumptions about initial precursor concentrations, emission patterns, dilution, transported pollutants, reactivity, and light intensity are incorporated in each simulation.

Ozone Isopleth Diagram

An ozone isopleth diagram shows curved isolines linking constant, maximum, one-hour average ozone concentrations as a function of the VOC and NO_x emissions that were predicted to have produced these concentrations. An isopleth generated by OZIPM-4 is illustrated in Figure 1. The NMOC and NO_x coordinates associated with any point on a single, curved isoline produced the same maximum concentration of ozone during simulations. In OZIPM-4, 121 simulations are normally performed to produce such a diagram.

Reactivity

This is a property of the precursors that governs the rate and extent of ozone production. In general, a more reactive organic compound or mixture will produce more ozone, or produce ozone more rapidly than a less reactive compound or mixture. Different kinetic mechanisms will represent reactivity differently.

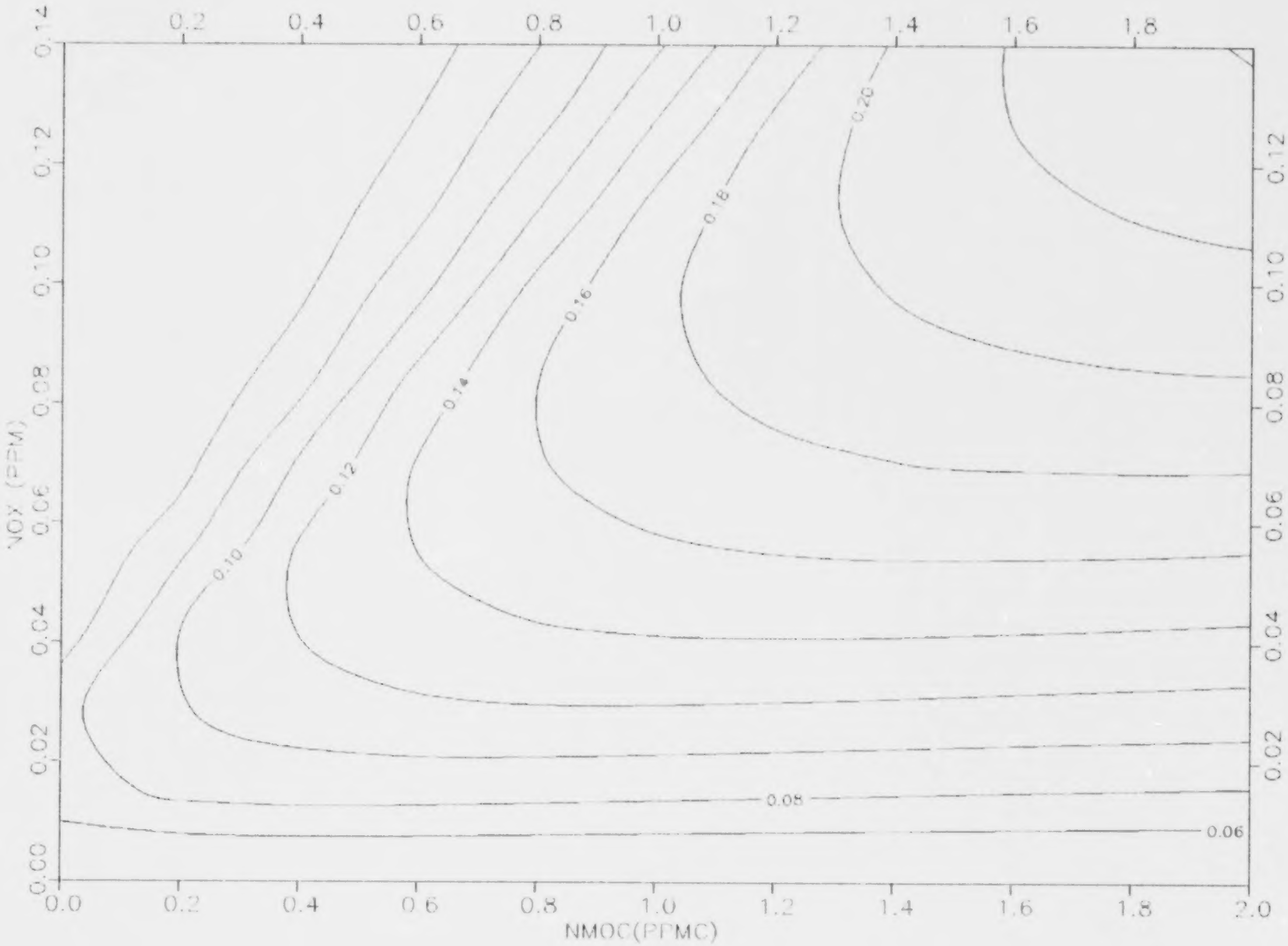

FIGURE 1. Example ozone isopleth diagram (curved lines are constant, predicted, maximum hourly ozone concentrations (pphm) for the VOC and NO_x precursor concentrations on each axis).

Default Values

Certain parameters are needed to run OZIPM-4. The default values are the values of these parameters that will be used unless other values are entered in the input data. For example, the default value for the highest NMOC used in the construction of an isopleth diagram is 2.0 ppmC. If no number is entered in the input data for this parameter, OZIPM-4 will use 2.0 by default.

Diagram Point

Any point on an ozone isopleth diagram is associated with three concentrations: initial NMOC and NO_x precursor concentrations, and a maximum one-hour average ozone concentration corresponding to the initial NMOC and NO_x levels. A set of these three parameters is termed a diagram point. The ozone concentrations at some diagram points are determined from actual computer simulations, while the ozone concentrations at intermediate diagram points are interpolated from the concentrations at the simulated diagram points.

Spline Interpolation

Spline interpolation is used to determine the ozone concentrations between diagram points for which ozone concentrations have been calculated by computer simulations. A spline function is similar to a wire constrained to touch certain points. If the wire is pulled taut, it will bend at each point, but will be straight between points. If the tension is reduced, the wire will provide a smooth curve that touches the points. The hyperbolic spline functions used to interpolate between calculated diagram points in OZIPM-4 have an adjustable tension factor analogous to the tension on a wire. Interpolations are performed internally by the OZIPM-4, and usually there is no need for the user to be directly concerned with the spline functions.

SUMMARY OF INPUT DATA

Input parameters that can be specified by the user when performing an OZIPM-4 calculation include:

A new chemical kinetic mechanism;

The zenith-angle-dependence of the photolysis rates in the chemical mechanism;

Latitude;

Longitude;

Time zone;

Date;

Morning and afternoon mixing heights (also called mixing depths) or hourly mixing depths;

Hourly temperature variation;

The simulation start and stop times;

Concentrations of NMOC, NO_x, CO, ozone, and up to 10 other species in the air above the mixed layer due to transport aloft (note that these cannot be varied in time);

Concentrations of NMOC, NO_x, CO, ozone, and any other chemical species transported in the surface layer;

Background concentrations of NMOC, NO_x, and ozone. The background represents the minimum levels in both the surface layer and aloft that could be achieved if all urban emissions were reduced to zero (i.e., continental background);

VOC, NO_x, and CO emissions at each hour;

Organic reactivity. Four reactivities can be specified: background, initial, aloft, and emitted. However, each type of reactivity is fixed in time for each diagram point and at every point on the diagram;

NO_x reactivity (initial fraction of NO_x that is NO_2);

Surface deposition as a function of time for up to 10 species.

OUTPUT OPTIONS

The major function of OZIPM-4 is to estimate the NMOC reductions needed to achieve the ozone air quality standard. The output depends on the option selected by the user. Three types of output can be requested:

(1) Perform a single calculation for a specified set of initial concentrations.

(2) Compute VOC emission reduction needed to achieve the O_3 standard of 0.12 ppm without generating an O_3 isopleth.

(3) Generate an O_3 isopleth.

In addition, the user may generate isopleths for species other than ozone and perform off-line (CALCOMP) plotting.

SECTION 2

TECHNICAL DISCUSSION

The OZIPM-4 is a trajectory-type model designed to simulate ozone formation in urban atmospheres. The model consists of two distinct components: The first is a trajectory-based kinetic simulation model that mathematically simulates the physical and chemical processes taking place in the atmosphere; the second uses the simulation results to calculate a control strategy for a specific test case or to construct an ozone isopleth diagram. This section describes the conceptual basis of the kinetics model and the mathematical techniques used to perform a simulation.

CONCEPTUAL BASIS FOR THE OZIPM-4 KINETIC MECHANISM

In the OZIPM-4 kinetics model, a column of air containing ozone and precursors is transported along an assumed trajectory. As the column moves, it encounters fresh precursor emissions that are uniformly mixed within the column, which is assumed to extend from the earth's surface through the mixed layer. The assumed horizontal dimensions of this column are such that the concentration gradients are small enough to make the horizontal exchange of air between the column and its surroundings insignificant. The air within the column is assumed to be uniformly mixed at all times.

At the beginning of a simulation, the column is assumed to contain some specified initial concentrations of NMOC and NO_x. As it moves along the assumed trajectory, the height of the column can change because of temporal and spatial variations in mixing height; it is assumed to change with time during a user-selected period, and to be constant before and after that period. As the height of the column increases, its volume increases, and air above from the inversion layer is mixed in. Pollutants above the mixed layer are described as "transported above the surface layer" or "transported aloft." Any ozone or ozone precursors above the mixed layer that are mixed into the column as it expands are assumed to be rapidly mixed throughout the column.

The kinetics model in OZIPM-4 also considers emissions of VOC, NO_x, and CO into the column as it moves along its trajectory. The concentrations of these species within the column are physically decreased by dilution due to the inversion rise, and physically increased both by entrainment of pollutants transported aloft and by fresh emissions. All species react chemically according to the kinetic mechanism selected. Certain photolysis rates within that mechanism are functions of the intensity and spectral distribution of sunlight, and they vary diurnally according to time of year and location.

The following assumptions and specifications describe the OZIPM-4 trajectory model:

> The air mass of interest is an imaginary air parcel (column) of fixed horizontal area at a diurnally varying uniform temperature, within which pollutants are well mixed.
>
> The region of the atmosphere containing the imaginary column is sufficiently homogeneous that horizontal diffusion does not affect pollutant concentrations within the column.
>
> The height of the column varies with time as specified by the user.
>
> The column contains specified initial concentrations of NMOC, NO_x, and CO at the simulation starting time.
>
> Pollutants transported within the surface layer from outside the area of interest may be present in the column at the beginning of each simulation. The pollutant concentrations due to transport in the surface layer are normally assumed to be zero, but the user can specify other values for the NMOC, NO_x, CO, and ozone concentrations transported within this layer.
>
> Changes in pollutant concentrations within the column are calculated by computer simulation for a user-specified period.
>
> Entrainment of pollutants transported aloft is possible during the rise of the mixed layer. OZIPM-4 permits entrainment of NMOC, NO_x, ozone, and a limited number of other species, but the concentrations in the layer aloft cannot be varied in time.
>
> Pollutants emitted into the column after the starting time can be represented by specifying additions of VOC, NO_x, and CO, and other species during each hour.
>
> Zero cloud cover is assumed.

Other assumptions relating to the use of EKMA to predict control requirements or changes in urban ozone concentrations as a result of changes in precursor emissions are discussed in EPA (1981).

COMPUTATIONAL PROCEDURES

This section presents a detailed description of the mathematical procedures used in OZIPM-4 to calculate the maximum one-hour average ozone concentration that results from given initial concentrations of NMOC and NO_x. These procedures are based on the physical and chemical processes described in the last section. Before the beginning of a simulation, data-preparation steps are performed by the program. A simulation is conducted by first determining concentrations at the starting time and then numerically integrating the equations that form the basis of the model. The numerical solution continuously yields species concentrations as a function of time throughout the simulation period. The following discussion describes the data-preparation steps, the calculation of initial concentrations, the model formulation, and the numerical integration technique used.

Data-Preparation Steps

Because all simulations performed by OZIPM-4 in generating an ozone isopleth diagram have identical conditions except for the initial NMOC and NO_x concentrations, a data-preparation step is performed by the program before the first simulation begins. The purpose of this step is to eliminate abrupt changes in photolytic rate constants and emission rates. Elimination of these abrupt changes (i.e., discontinuities) is desirable for three reasons:

(1) The integration scheme requires less computer time (discontinuities require the use of small time steps).

(2) The results are more accurate numerically (stepping past discontinuities without preparation can lead to errors).

(3) The atmosphere does not normally have discontinuities. (The simulation of intermittent cloud cover or sudden changes in emissions is outside the scope of OZIPM.)

The solar zenith angle is evaluated every hour using an algorithm developed by Schere and Demerjian (1977). The algorithm uses latitude, longitude, time zone, and date as input data to calculate photolytic constants. A set of third-order polynomial spline functions is then generated so that the photolysis rate of NO_2 (based on the calculations of Jeffries, Sexton, and Arnold, 1987) can be calculated from a smooth curve for any time of the day. At a given zenith angle, all other photolysis constants used in OZIPM-4 are assumed to be either proportional to the NO_2 photolysis rate or a function of the zenith angle when specified explicitly by the user.

Emission rates are expressed either as fractions of the initial precursors or as emission densities for each hour. The emission rates are converted to continuous functions for use in solving the differential equations through a histogram-fitting algorithm described by Jeffries, Sexton, and Salmi (1981). The histogram-fitting algorithm replaced the spline-fitting algorithm described in the original OZIPP manual because the latter yielded widely oscillating functions.

Determination of Initial Concentrations

Before a simulation can begin, the concentrations of all pollutant species at the starting time must be determined by the program. These concentrations are derived from the initial concentrations of NMOC and NO_x that are specified by the user. The concentrations of transported pollutants are assumed to be zero unless otherwise specified by the INITIAL, ALOFT, TRANSPORT or BACKGROUND options (see Section 3).

The concentrations of the nonzero species are determined by the program in the following manner:

(1) NO_2 is set to the initial NO_x concentration multiplied by the NO_2/NO_x fraction (NO_2/NO_x fraction default is 0.25).

(2) NO is set to the initial NO_x concentration multiplied by the quantity one minus the NO_2/NO_x fraction.

(3) O_3 is set to the concentration transported in the surface layer or to the background value, whichever is larger (default is zero).

(4) The concentrations of the organic species are determined from the assumed initial NMOC concentration and the assumed reactivity fraction. Mathematically,

$$[\text{organic}]_i = [\text{NMOC}]\ (R_i)/C_i \tag{2-1}$$

where

$[\text{organic}]_i$ = the concentration of the i-th organic species in ppm

$[\text{NMOC}]$ = the concentration of the initial NMOC concentration, ppmC

R_i = carbon fraction of initial NMOC that is species i

C_i = number of carbon atoms in species i

(5) Two species (H_2O and carbon monoxide) are set at nonzero concentrations if they are not explicitly entered by the user. H_2O is set to a concentration of 20,000 ppm and carbon monoxide is set to 1.2 ppm initially, and 0.5 ppm aloft (Baugues, 1987).

Mathematical Formulation of Concentration Change Processes

The kinetics model in OZIPM-4 mathematically simulates physical and chemical processes taking place in the atmosphere. This simulation is accomplished by numerically integrating a system of ordinary differential equations that describe the effects of these processes on pollutant concentrations. The result gives the concentration of pollutants as a function of time. The mathematical formulation of the system of differential equations is described next.

In OZIPM-4, five processes are assumed to affect pollutant concentrations:

(1) Chemical reactions
(2) Dilution
(3) Entrainment of pollutants transported aloft
(4) Emissions
(5) Surface deposition

Differential equations are used to describe the time rate of change of pollutant concentrations due to each process. The total time rate of change of each pollutant concentration is then simply equal to the sum of all these effects. Thus, the system of equations consists of one differential equation for each species in the kinetic mechanism. The five processes are described next.

Chemical Reaction Effects--

The change in pollutant concentration due to chemical reaction is a function of the rates of the chemical reactions. The rate of each reaction is the product of a rate constant and a concentration of each reacting species. The photolytic rate constants are calculated by procedures that will be described later. The concentration term for unimolecular or pseudo-first-order reactions (such as photolytic reactions) is simply the concentration of the reactant. Bimolecular reaction rates are calculated similarly, except that the concentration term is the product of the two reactant concentrations. For example, the reaction rate (RT) for the reaction,

$$NO + O_3 \rightarrow NO_2 + O_2, \tag{2-2}$$

would be expressed as

$$(RT)_2 = k_2\, C_{NO}\, C_{O_3}$$

where

$(RT)_2$ = rate of reaction 2, ppm min^{-1}

k_2 = rate constant for reaction 2, $\text{ppm}^{-1}\ \text{min}^{-1}$

C_{NO} = concentration of NO, ppm

C_{O_3} = concentration of O_3, ppm

If the rate constant varies as a function of temperature, then k_2 would be represented by the rate constant at 298 K, along with an activation energy term (E/R), in degrees K, such that

$$k_2 \text{ (at temperature T)} = k_{298} \times \exp\left[E/R\left(\frac{1}{298} - \frac{1}{T}\right)\right] \quad .$$

The time rate of change of a species due to chemical reaction is simply equal to the sum of all rates for those reactions in which the species is a product minus the sum of the rates for those reactions in which the species is a reactant. Thus,

$$\left(\frac{dC_i}{dt}\right)_R = \Sigma\ (RT)_{PROD} - \Sigma\ (RT)_{REAC} \tag{2-3}$$

$\left(\frac{dC_i}{dt}\right)_R$ = chemical reaction contribution to the time rate of change of species i

$\Sigma(RT)_{PROD}$ = the sum of all reaction rates in which species i appears as a product

$\Sigma(RT)_{REAC}$ = the sum of all reaction rates in which species i appears as a reactant

Dilution Effects--

The mathematical representation for simple dilution due to changes in the mixing depth is a first-order decay process. The rate of change due to this effect can be represented as follows:

$$\left(\frac{dC_i}{dt}\right)_D = -DC_i \tag{2-4}$$

where

$\left(\frac{dC_i}{dt}\right)_D$ = dilution effect contribution to the time rate of change of pollutant species i, ppm min^{-1}

D = dilution factor, min^{-1} (function of time)

C_i = concentration of species i, ppm

The dilution factor is calculated in one of two ways depending on the option chosen: The first method of dilution assumes that the mixing height varies from a minimum (or morning) mixing height to a maximum (afternoon) mixing height in accordance with a "characteristic curve" derived empirically from data taken during the St. Louis RAPS study (Schere and Demerjian, 1977). The "characteristic curve" represents the fractional growth in mixing height as a function of the fraction of daylight. The fraction of daylight is calculated as follows:

$$\text{Fraction of daylight} = \frac{\text{Time (current)} - \text{(time of sunrise)}}{\text{(time of sunset)} - \text{(time of sunrise)}}$$

The mixing height at any given time is

$$\text{Mixing height} = H_o + F_G \times \Delta H$$

where

H_o = mixing height at time of sunrise (calculated from the minimum mixing height)

ΔH = maximum mixing height - H_o

F_G = fraction of growth in mixing height.

The "characteristic curve" is depicted graphically in Figure 2. Note that before and after the inversion rise period, the dilution factor is zero since there are no dilution effects for those periods.

Two modifications were made to the characteristic curve concept to facilitate its use. First, a smooth curve through the points shown in Figure 2 was used to avoid discontinuities. Second, the mixing height at the start of the simulation (usually 0800 hours) was used instead of H_o as noted above since most simulations start after sunrise.

The second method of dilution is the specification of hourly mixing heights. When hourly mixing depths are specified, the dilution factor at each time step is calculated in the following manner:

$$D_t = \dot{H}/H_t$$

where

D_t = dilution factor at time t, min^{-1}

$\dot{H}$ = the rate of change in mixing depth with time at time t, length min^{-1}

H_t = mixing depth at time t, length.

Entrainment Effects--

Pollutants above the mixed layer are subject to entrainment. In OZIPM-4, these are limited to NMOC, NO_2, O_3, CO, and up to 10 other chemical species. The mathematical treatment of entrainment assumes that

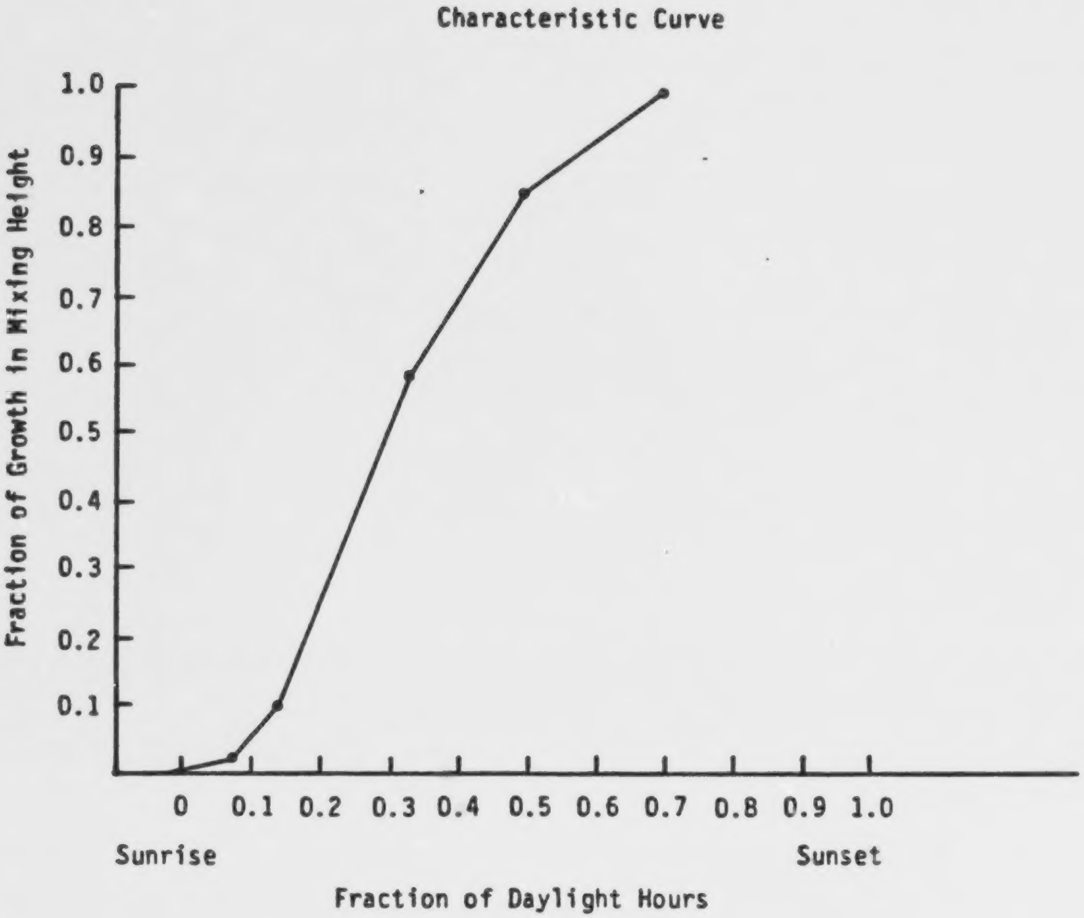

Figure 2. Graphical depiction of mixing height "characteristic curve."

the concentrations aloft do not change with time and that they extend uniformly to at least the height of the afternoon mixed layer. The pollutants entrained are assumed to mix rapidly within the enlarged surface layer. The mathematical expressions for the rates of change of the pollutants are shown by the following equations:

$$\left(\frac{dC_i}{dt}\right)_{AL} = D_t(C_i)_{AL} \tag{2-5}$$

$$\left(\frac{dC_{HC_j}}{dt}\right)_{AL} = D_t(C_{NMOC})_{AL}\ R_{HC_j}\ /C_j \ , \tag{2-6}$$

where

$\left(\frac{dC_i}{dt}\right)_{AL}$, $\left(\frac{dC_{HC_j}}{dt}\right)_{AL}$ = the contribution of entrainment to the time rates of change of species i or hydrocarbon species j, respectively, ppm min^{-1}

D_t = dilution factor (i.e., the rate constant at time t for the mixing height rise), min^{-1}

R_{HC_j} = carbon fraction of the C_{HC_j}

$(C_i)_{AL}$ = concentration of ozone, NO_2, and up to 10 other species trapped aloft, ppm

$(C_{NMOC})_{AL}$ = concentration of total nonmethane organic compounds trapped aloft, ppmC

C_j = number of carbon atoms in species j

It should be noted that the effect of the change in mixing height is the sum of the dilution and the entrainment effects.

Emission Effects--

Emissions are the fourth factor affecting the rate of change of pollutant concentrations. The rates of change due to emissions are equal to the additional concentrations produced by the emissions. Because equal moles of emissions into different volumes will produce different concentrations, it is necessary to adjust the relative emissions to reflect the change in the column volumes due to the inversion rise. This is done internally in OZIPM-4 by first calculating the ratio of the starting inversion height to the current inversion height. (This is equivalent to the ratio of initial volume to the current volume.) Before the inversion rise begins, this ratio is one. After the inversion rise has ceased, the ratio is the initial mixing height divided by the final mixing height. In general, the ratio (ft) is the ratio of the initial mixing height to the mixing height at time t.

The rates of change due to the emissions are calculated from the values of the emission rates (calculated using the interpolating functions described earlier), the f_t ratio just described, and the reactivity inputs. The equations for the rates of change due to emissions for each of the affected species are shown below:

$$\left(\frac{dC_i}{dt}\right)_E = f_t(E_i)_t \quad ,$$

where

$\left(\frac{dC_i}{dt}\right)_E$ = emission contribution to the rates of change of species i, ppm min^{-1}

$(E_i)_t$ = value of emission rate of species i, ppm min^{-1}

For these formulations, a conversion from ppmC to ppm is performed for hydrocarbon species, and the reactivity of the hydrocarbons is taken into account.

The normal emissions input to OZIPM-4 is in fractions of initial NMOC and NO_x concentration, which gives ppm or ppmC emission rates. Other emissions options in OZIPM-4 allow the user to input mass or molar emissions rates. Molar emissions input to OZIPM-4 must be converted to normalized ppm units for the amount to be added each hour. The different emissions options available will automatically convert the emission density from moles $m^{-2}hr^{-1}$ to the required units; these options are discussed in Section 3. To convert emissions of moles $m^{-2}hr^{-1}$ to ppm/hr, one multiplies by 24450 $moles^{-1}$ for each hour and divides by the initial mixing height m to normalize the values.

Carbon monoxide emissions can be treated explicitly using a new option (CREDIT) discussed in Section 3.

Surface Deposition Effects--

The deposition rate is a function of surface type and the individual species' resistence to surface uptake. In general, NO, NO_2, and O_3 have high deposition rates, whereas organic compounds have very low deposition rates. Species surface deposition can be treated in a manner similar to that for dilution. In OZIPM-4 the rate of surface deposition is equal to the deposition velocity (in units of cm/s) times the pollutant concentration divided by the height of the mixed layer. Thus, the rate of change of the pollutants can be expressed as:

$$\left(\frac{dC_i}{dt}\right)_{\text{Deposition}} = - V_d \times C_i \div H \times 0.6$$

where V_d is the deposition velocity in units of cm/s, and H is the height of the mixed layer (m), and 0.6 is the conversion from cm/s to m/min.

Description of Numerical Integration

The kinetics model in OZIPM-4 employs a Gear-type integration scheme to numerically solve the set of differential equations described in the previous section. A detailed description is not given here because the method is not unique to OZIPM-4, and the procedure has been described elsewhere (Gear, 1971; Spellman and Hindmarsh, 1975; Sherman, 1975). The integration scheme initially uses a time step of 1×10^{-10} minutes (i.e., pollutant concentrations are to be calculated 1×10^{-10} minutes after the start time). Subsequent time step sizes are then computed by the Gear type integration scheme according to the estimated error at each step. The pollutant concentrations are calculated at each time step throughout the simulation period. (Once the final hour is reached, there is no restriction on precisely matching the final time step, since the concentrations can be interpolated back to exactly the last hour.) A typical simulation period takes from 150 to 200 time steps; about one-half of these time steps are used in simulating the first minute.

The total rate of change of any species is the sum of the rates of change due to dilution, entrainment, emissions, surface deposition, and chemical reaction just described. At each time step, the concentrations of all species are calculated along with the current rates of change for each species to predict the species concentration at the end of the time step using a Taylor-series type polynomial. The order of the polynomial is varied internally for optimum efficiency and is based on the values at the beginning of the time step. A corrective scheme then "corrects" the new concentration values, updates the Taylor polynomials, and estimates the average error. The corrector is a set of linear equations based on a Jacobian matrix whose elements are the set of partial derivatives of rate of change of concentrations of each species with respect to each of the other species. OZIPM-4 utilizes a linear system solving package for sparse matrices (i.e., those matrices in which most elements are equal to zero).

The integration method used in OZIPM-4 has been modified somewhat from the version published by Spellman and Hindmarsh (1975). For example, the error estimation is performed relative to the current concentration of a species rather than relative to its maximum concentration. The method utilizes the error estimate to determine the optimum step size and order, so that the allowable error specified by the user is met with the minimum number of integration steps.

The final task performed during the integration of the differential equations is determination of the maximum one-hour-average ozone concentration. Ozone concentrations are calculated for every minute of the simulation. This calculation is performed by interpolation between the actual time steps used in the integration. Running one-hour average concentrations are calculated using Simpson's rule and are updated every minute. The largest one-hour average concentration is then selected as the maximum.

GENERATION OF ISOPLETH DIAGRAMS

It is not necessary to use isopleth diagrams to perform EKMA calculations with the EKMA option in OZIPM-4. However, though use of the EKMA option will provide the target VOC control requirements, in some cases, an isopleth diagram can provide additional diagnostic information. These circumstances include:

> The occurrence of a maximum (or maxima) along the line of constant NMOC/NO_x ratio leading to two or more design ozone points (or a maximum lower than the design ozone).

A design ozone that does not fall on the line of constant NMOC/NOx ratio.

The program cannot find the 0.12 ppm (NAAQS) ozone level.

The program cannot find the design ozone concentration within 8 trys.

The use of an isopleth diagram to develop a better understanding of the characteristics of the isopleth curves.

For situations that require an isopleth diagram, the user specifies the maximum NMOC and NO_x concentrations, respectively, for the abscissa and ordinate. The OZIPM-4 performs a series of 121 simulations to generate predicted ozone concentrations on an 11 x 11 (NMOC x NO_x) rectangular grid with points evenly spaced within the specified maxima. From these 121 simulations, the pollutant isolines are estimated based on contouring procedures described by Sutcliffe (1978). The contouring procedures are based on a tracing algorithm that searches the rectangular grid of data points and finds the diagram point with a value just greater than the isoline of interest. An interpolation is then performed at the interval of interest using a hyperbolic spline interpolation scheme developed by Cline (1974).

The algorithm proceeds through the rectangular grid tracing the isoline from one edge of the diagram to another edge (Figure 3). The four outer edges of the rectangular grid beginning on the bottom edge and moving counterclockwise are scanned until an interval containing the desired isoline is found. In the example shown in Figure 3, the isoline begins on the left edge (edge 2). The first point is the point with a value just greater than the isoline value (point 1). At point 1, a clockwise sweep of the surrounding eight points (5 points, when the center point is an edge point) determines (1) which interval the isoline intersects (horizontal or vertical), the center point, and the neighboring point and (2) where the center point will be for successive scans. The tracing procedure is continued until an edge is again reached.

The intersection of the isoline at some point on the interval between the center point and the neighboring point (points 1 and 1' on Figure 3) is determined by a spline interpolation scheme that uses all the data points along the vertical or horizontal line. Thus, in Figure 3, all data points along the left edge are used to determine the intersection of the isoline with some point on the interval from point 1 to 1'. The interpolation scheme is repeated for each successive center point. In Figure 3, at point 13, all data points along the horizontal line containing points 13 and 13' are used to determine the intersection of the isoline with some

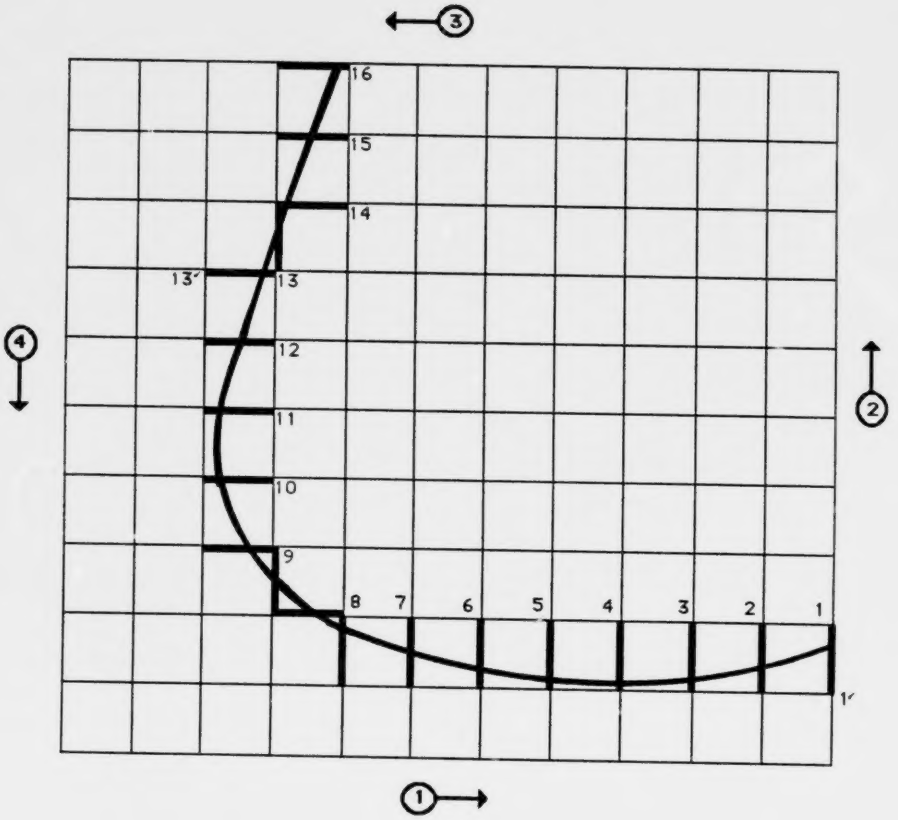

FIGURE 3. Illustration of the tracing procedures used to construct an isopleth diagram.

point on the interval between points 13 and 13'. The use of spline interpolation is an improvement over the use of strict linear interpolation within the interval of interest. The tracing procedure is repeated for each isoline value specified by the user or by the default set stored within the OZIPM-4 program.

SECTION 3

DESCRIPTION OF OZIPM-4 OPTIONS

This section contains detailed description of the different options and inputs available for use with the OZIPM-4 computer code. Currently, there are 26 options. The first four letters of each option have been underlined to denote the required input code. Briefly, these options are:

Optional Mechanism Input:

MECHANISM - input a different chemical kinetic mechanism

ZENITH - input zenith angle dependence of the photolytic rate constants for optional mechanism or revise zenith angle dependence for the default mechanism

City-Specific Inputs:

PLACE - location of the site

DILUTION - input minimum and maximum inversion heights

MIXING - input hourly inversion heights

TEMPERATURE - input hourly temperature values

DEPOSITION - input hourly surface deposition rates for specified species

TRANSPORT - input surface layer and aloft conditions of NMOC, NO_x, and O_3

INITIAL - input conditions of species transported in the surface layer other than NMOC, NO_x, and O_3

ALOFT - input aloft conditions of species other than NMOC, NO_x, and O_3

BACKGROUND - input background conditions of NMOC, NO_x, and O_3

EMISSIONS - input hourly emission fractions of VOC and NO_x

MASSEMISS - input hourly mass emission densities of VOC and NO_x

MOLEMISS - input hourly molar emission densities of up to 5 species

REACTIVITY - input reactivity of the initial NMOC mix and VOC emissions and the initial NO_2/NO_x ratio

CREDIT - input hourly emission fraction (or emission densities) of carbon monoxide (CO) and allow for change in CO in the future year

Additional Simulation Options:

TITLE - input simulation title

TIME - input starting and ending times for computer simulations

RATE - change chemical reaction rate constants (for testing purposes)

SPECIES - input the species of interest for isopleths

ACCURACY - change the accuracy of the simulation (error tolerance) and the tolerance for spline interpolation

ALREADY - time saving option utilizing simulations from a previous run

PLOT - perform off-line plotting (CALCOMP)

Program Output Options:

EKMA - calculate VOC reductions needed to achieve the O_3 standard of 0.12 ppm

CALCULATION - conduct a single simulation for a specified pair of initial NMOC and NO_x concentrations

ISOPLETH - construct an isopleth plot

The following dicussion describes the use of these options. Also, recall that Section 5 describes the specific format requirements for each option discussed here.

CHEMICAL KINETIC MECHANISM

As noted earlier, the CBM-IV is internally stored in the OZIPM-4 program. However, the program has the capability to accept a chemical mechanism other than the default CBM-IV. This optional kinetic mechanism cannot contain more than 135 reactions and/or 60 species. To input a different kinetic mechanisms, the user must specify certain parameters:

> The total number of photolysis reactions (maximum of 20) and the reaction numbers that identify the photolysis reactions in the mechanism.
>
> The total number of organic species included in the initial NMOC mix (maximum of 20), the names that identify these species, and the number of carbon atoms in each.
>
> The fraction of total carbon that each organic species represents.

The following subsection discusses how mechanisms are coded into OZIPM-4.

Input of an Optional Mechanism

An optional mechanism is processed with the MECHANISM option code. After MECHANISM is entered the following parameters are specified: the reaction identification number of the last reaction to be read, the total number of photolysis reactions, the total number of organic species in the initial mix, the mechanism input format, and the temperature. The program will then read the following line(s) in the following order:

> The list of photolysis reactions (up to seven on a line, twenty reactions maximum).
>
> The list of names for the organic species that are included in the initial NMOC mix (up to seven to a line, 20 species maximum).
>
> The list of carbon numbers for the organic species in the same order as above.

After the list of carbon numbers for the species is read, the mechanism itself is input. Each reaction is input on a separate line. Note that the species names used in the kinetic mechanism must be consistent (e.g., HO and OH will represent different species).

There are currently two input formats for chemical reactions. The first format is similar to the formatting used in the CHEMK chemical kinetics program developed for the EPA (Whitten and Hogo, 1980). This format is provided for users who have chemical mechanisms already set up for the CHEMK program. The CHEMK format allows for up to 3 reactants and 4 products per input line. Stoichiometric coefficients of one are assumed. As an example, the reaction $2NO + O_2 \rightarrow 2NO_2$ must be written in the following form: $NO + NO + O_2 \rightarrow NO_2 + NO_2$.

CHEMK Reaction Input

Each CHEMK-type reaction line allows input of the reaction identification number, up to three reactants, up to four products, the rate constant at 298 K, and the activation energy in degrees Kelvin. Since the stoichiometric coefficients for all reactants and products in each reaction are ignored in the CHEMK format, the user will need to rewrite certain reactions when using this format. The following reaction provides an example:

$$RCHO + h\nu \rightarrow 0.5\ RO_2 + 1.5\ HO_2 \qquad k_3 = 0.0025\ \text{min}^{-1} \qquad (3\text{-}3)$$

This reaction must be written so that all stoichiometric coefficients are equal to one. This can be done by separating the reaction into several reactions such that the sum of the new reactions will be equal to the original reaction (3-3) at the same overall rate for all species.

In general we start with the form

$$A + B + C \rightarrow X_1D + X_2E + X_3F \qquad k_4 \qquad (3\text{-}4)$$

where the Xs are fixed such that

$$0 \le X_1 \le X_2 \le X_3 \le 1.0\ .$$

For the example case [Reaction (3-3)]

$$RCHO + h\nu \rightarrow 0.5\ RO_2 + 0.5\ HO_2 + 1.0\ HO_2 \qquad (3\text{-}3)$$

the general Reaction (3-4) can be rewritten as four reactions:

$$A + B + C \rightarrow D + E + F \qquad k_5 \qquad (3\text{-}5)$$

$$A + B + C \rightarrow E + F \qquad k_6 \qquad (3\text{-}6)$$

$$A + B + C \rightarrow F \qquad k_7 \qquad (3\text{-}7)$$

$$A + B + C \rightarrow \qquad k_8 \qquad (3\text{-}8)$$

where $k_4 = k_5 + k_6 + k_7 + k_8$ and the rate constants for Reactions (3-5) through (3-8) are defined as follows:

$$k_5 = X_1 k_4$$

$$k_6 = (X_2 - X_1)k_4$$

$$k_7 = (X_3 - X_2)k_4$$

$$k_8 = (1 - X_3)k_4$$

Using this scheme for the example Reaction (3-3), the four reactions are

$$RCHO + h\nu \rightarrow RO_2 + HO_2 + HO_2 \qquad k_9 \qquad (3\text{-}9)$$

$$RCHO + h\nu \rightarrow HO_2 + HO_2 \qquad k_{10} \qquad (3\text{-}10)$$

$$RCHO + h\nu \rightarrow HO_2 \qquad k_{11} \qquad (3\text{-}11)$$

$$RCHO + h\nu \rightarrow \qquad k_{12} \qquad (3\text{-}12)$$

Rate constants for these reactions are

$$k_9 = 0.5k_3$$

$$k_{10} = (0.5 - 0.5)k_3 = 0$$

$$k_{11} = (1.0 - 0.5)k_3 = 0.5k_3$$

$$k_{12} = (1.0 - 1.0)k_3 = 0$$

Therefore, only Reactions (3-9) and (3-11) are needed to represent Reaction (3-3), both reacting with $k = 0.00125\ \text{min}^{-1}$. Note that the sum of Reactions (3-9) and (3-11) is

$$\begin{array}{ll} RCHO + h\nu \rightarrow RO_2 + HO_2 + HO_2 & (3\text{-}9) \\ \underline{RCHO + h\nu \rightarrow HO_2} & (3\text{-}11) \\ 2RCHO + 2h\nu \rightarrow RO_2 + 3HO_2 & \end{array}$$

which is the same as Reaction (3-3). The general scheme outlined here applies to all reactions that can be transformed into the form of Reaction (3-4).

EPASIM Reaction Input

The second format for the chemical reactions allows the user to input nonunity stoichiometric coefficients for the products of the reaction. This format is an extension of the chemical mechanism input format for the EPASIM chemical kinetics computer program (Overton, 1976). This format also allows the user to input up to nine products. For example the reaction

$$\begin{aligned} EL + NO \rightarrow 3\ NO_2 - 2\ NO + 0.5\ HO_2 + 0.5(CHO)_2 + 0.5\ CH_3CO_3 \\ + 0.5\ CH_3COCHO + 0.5\ CO \end{aligned}$$

can be input as follows:

(1) EL + NO → 3 NO2 - 2 NO + 0.5 HO2

(2) + 0.5 CHO2 + 0.5 ETO3 + 0.5 ALLE + 0.5 CO

where the numbers on the left side represent the line input sequence. Note that four character symbols are used in place of the actual species symbols. Each chemical reaction line contains up to three reactants, the reaction identification number, up to three products (with the associated stoichiometric coefficient), the rate constant at 298 K, and the activation energy in degrees Kelvin. If the reaction contains more than three products, the extra products are input in a continuation line following the first line, provided that a flag was placed in the first line to denote the continuation sequence.

The required format for this and the CHEMK reaction input lines is explained in Section 5. For both formats the last reaction must have a reaction number corresponding to the number given on the MECHANISM line, though it need not be the highest reaction number in the mechanism. Rate constants must be in min^{-1} for unimolecular reaction, in $ppm^{-1}min^{-1}$ for bimolecular reactions, and in $ppm^{-2}min^{-1}$ for termolecular reactions. The units of the activation energy (if used) must be in degrees Kelvin (K).

Photolysis reactions can be treated in one of two ways when inputting an optional mechanism into OZIPM-4:

(1) The rate of photolysis for a particular species can be assumed to vary with zenith angle in a fashion similar to NO_2. The rate constant for photolysis in such a case would then be expressed as some constant multiple of the rate constant for photolysis of

NO_2. The user would designate the specific reaction as a photolysis reaction (using the MECH option) and input this multiple in the rate constant slot for that reaction. For example, if it is assumed that the photolysis of HNO_2 proceeds at a rate equal to 0.1975 times the rate of photolysis of NO_2, the user would include the HNO_2 photolysis reaction number as a photolysis reaction and input a value of 0.1975 in the rate constant field of the reaction line for HNO_2 photolysis.

(2) The rate of photolysis for a particular species can be varied with zenith angle in a fashion that is not similar to NO_2. In this case, the user should input a value of 1.0 in the location on the reaction line where the rate constant is placed. The user would then use the ZENITH option to input (as a function of zenith angle) the photolysis ratios relative to NO_2 for the species of interest. That is, one does not input the absolute rates; but rather, a relative rate that, when multiplied by the NO_2 photolysis rate for that zenith angle, will yield the desired absolute rate. The ZENITH option is discussed in detail later in this subsection. Again, the reaction of interest must be identified as a photolysis reaction with the MECHANISM option.

Photolytic rate constants for NO_2 as a function of zenith angle are stored internally in OZIPM-4. Normally, when inputting a mechanism, the user would place a value of 1.0 in the rate constant field of the reaction line for NO_2 photolysis. The user, however, has the option to change the photolysis rate for this species. For example, to perform simulations with a 10 percent increase in the overall rate of NO_2 photolysis for all zenith angles, the user would input a value of 1.10 in the rate constant field of the NO_2 photolysis line. In addition, the user can use the ZENITH option to include a set of new values at different zenith angles (see below).

Modification of Rate Constants

Changes to any rate constant in the kinetic mechanism are made with the RATE option. On this line, the number of reactions with rate constant changes is placed in columns 11-20. If a nonzero number is entered in columns 21-30, a special option is activated in which all rate constants are set to zero except the photolysis rate constants. This allows the user to test the emissions, photolysis constants, and dilution rates. The photolysis rate constants can be set to zero with a PLACE option using a location above the arctic circle, near the winter solstice.

If only certain rate constants are to be changed, the first line after the RATE line contains the numbers of the reactions with rate constant changes (each located in separate 10-column fields; up to seven reaction numbers may be placed on a line). The next line(s) contains the new rate constants placed in the same location as that of the corresponding reaction numbers in the previous line(s).

ZENITH Option

Immediately following the MECHANISM option, the ZENITH option is used to revise or input photolysis rates as a function of zenith angles. In addition to those for NO_2, photolysis values for the following reactions are stored in OZIPM-4 as default values for the CBM-IV:

(1) $O_3 + h\nu \rightarrow O(^1D)$

(2) $FORM + h\nu \rightarrow 2\ HO_2 + CO$

(3) $FORM + h\nu \rightarrow CO$

(4) $ALD2 + h\nu \rightarrow XO_2 + 2HO_2 + CO + FORM$

(5) $H_2O_2 + h\nu \rightarrow 2OH$

(6) $OPEN + h\nu \rightarrow C_2O_3 + HO_2 + CO$

(7) $MGLY + h\nu \rightarrow C_2O_3 + HO_2 + CO$

Photolysis rates for these reactions are stored internally because these rates are known to vary with zenith angle in a fashion that is different from that of NO_2. Consequently, it would not be accurate to treat the photolysis of these species by coding a constant multiple of the NO_2 photolysis rate on the reaction lines as is done for the other photolysis reactions. For the first four reactions, separate zenith angle dependent values, are stored in the OZIPM-4 and rate constants of 1.0 are used in the mechanism. However, the inputs for the last three reactions are implemented differently because these functions depend on the functions for the second and third (formaldehyde) reactions. For H_2O_2 we use the zenith angle function of formaldehyde to stable products (reaction 3) and a rate constant ratio of 0.189. The OPEN and MGLY photolysis reactions use the zenith angle function of formaldehyde to radicals (reaction 2) and rate constant ratios of 8.40 and 8.96, respectively. The multiplication factors (0.189, 8.40, and 8.96) are entered in the rate constant field of the reaction line (see Gery, Whitten, and Killus, 1988, for a discussion of these rates).

When using the CBM-IV mechanism, the ZENITH option can be used to modify the default functions that are stored internally for the above species. It can also be used to consider the zenith angle dependency for other species that are presently assumed to photolyze in a manner similar to that of NO_2. The user would input his choice of the ratio to NO_2 photolysis for these reactions at zenith angles of 0, 10, 20, 30, 40, 50, 60, 70, 78, and 86 degrees. For example, if the user wishes to increase the NO_2 photolysis rate by 10 percent at a zenith angle of 0 degrees only, the user would input a value of 1.1 in Columns 11-20 of ZENITH option line 2. A value of 1.0 would be entered in the subsequent fields of the option lines. (The use of a ratio to NO_2 photolysis was chosen because many of the photolytic rate constants are reported as a ratio to NO_2 photolysis in the literature.) In addition, the rate constant of a photolysis reaction (input with the MECHANISM option) can be used as an overall correction factor to any zenith-angle-dependent function. Section 5 shows the format for the ZENITH option.

When the MECHANISM option is invoked, all photolysis reactions are assumed to vary as a function of zenith angle in a fashion similar to NO_2 photolysis. Thus, the ZENITH option must be used when an optional mechanism is input into OZIPM-4 if the photolysis reactions for species such as O_3, FORM, and ALD2 vary with zenith angle in a fashion that is different from the NO_2 photolysis.

When an optional chemical mechanism is used, the user must follow the procedures outlined here to ensure proper use of the photolysis reactions:

> The NO_2 photolysis reaction must be defined as the first reaction in the reaction list.
>
> All photolysis reactions will have an associated multiplication factor, which is input as the rate constant on the individual reaction line (in the MECHANISM option). This factor is an overall multiplier of the photolysis rate of interest.
>
> For those photolysis reactions that do not vary with zenith angle in a fashion similar to NO_2, the user must invoke the ZENITH option immediately after the MECHANISM option.
>
> Only those reactions that do not vary with zenith angle similar to NO_2 need be entered with the ZENITH option.

SITE-SPECIFIC INFORMATION

Up to 15 options can be used to describe the initial and meteorological conditions for the computer simulations. These options are PLACE, MIXING, DILUTION, TEMPERATURE, TRANSPORT, INITIAL, BACKGROUND, ALOFT, DEPOSITION, and TIME. Two different options, EMISSIONS (or MASSMOLE or MOLEMISS) and/or CREDIT can be used to describe emissions entering the air parcel during the simulation. The option REACTIVITY is used to specify site-specific information on the reactivity of the initial NMOC and NO_x ambient mix and the VOC and NO_x emissions.

Place and Date

In all OZIPM-4 runs, the rate constants of the photolysis reactions in the kinetic mechanism are varied in accordance with the diurnal change in sunlight intensity (or solar zenith angles) during the specified simulation period. This diurnal variation is calculated using a computer code written by Schere and Demerjian (1977) that is incorporated in OZIPM-4. The user can adjust the photolysis rate constants to the area of interest by changing the date or location, or both, from the default values of 21 June at Los Angeles, California. The option is activated by the code word PLACE. The first three numeric fields of the PLACE line (columns 11 through 40) contain the latitude (decimal degrees north), longitude (decimal degrees west), and time zone (hours from Greenwich Mean Time). The next three fields are used to specify the year, month, and day in columns 41-50, 51-60, and 61-70, respectively. An additional line may be required after the PLACE line if a nonzero value for the latitude or the longitude is entered. On this line, the name of the city of interest is entered between columns 1 and 24. Therefore, even if the default values of 34.058 and 118.250 specifically are entered, a second line is required. Users interested in the default location need not specify the latitude and longitude.

The numerical time zones for the continental United States is as follows:

Numerical Time Zone	Common Name
4.0	Eastern Daylight Time
5.0	Central Daylight Time
6.0	Mountain Daylight Time
7.0	Pacific Daylight Time

To produce standard time simulations, even though the output will show daylight time units, a false time zone can be created by incrementing the numerical time zone by one unit (hour). Thus, Pacific Standard Time photolysis constants would be generated if a 8.0 were entered instead of the 7.0 (daylight) time zone. The output should then show that solar noon occurs near 1200 hours when the printing of solar noon is activated.

Dilution Rate

Dilution in OZIPM-4 occurs as a result of the rise in the early morning inversion. Under default conditions, the inversion is assumed to rise from 510 meters to 630 meters over a 7-hour period starting at 0800 LDT using the characteristic curve.

City-specific values for determining the characteristic-curve dilution rate are entered using the word DILUTION. The values of the morning mixing height, afternoon mixing height, inversion rise starting time, and inversion rise stopping time are entered in the first four numeric fields of the DILUTION line (i.e., columns 11-20, 21-30, 31-40, and 40-50, respectively). The starting and stopping time should be in 24-hour time format, local daylight time. For both default and specific conditions, dilution is assumed not to occur outside the starting and stopping times.

Input of Hourly Mixing Heights

The second form of treating dilution in OZIPM-4 allows the user to input hourly inversion heights if such data are available or if the user does not want to use the characteristic curve to calculate the mixing height profile. The user declares this option (MIXING) and gives the number of hours dilution is to occur. The inversion heights are then entered for the initial height and for the end of each hour. Therefore, if there are n hours of dilution, n+1 inversion heights are entered. Dilution will always start at the beginning of a simulation (i.e., zero time). To have a zero dilution rate for a certain number of hours, the same inversion height should be given for those hours. Note that zero cannot be used as an inversion height. Up to 24 hours of dilution may occur (corresponding to 25 inversion heights). Any measure of length may be used to specify the mixing heights, but the unit of measure must be consistent for all values entered. The format for the MIXING option is given in Section 5.

Temperature

Another option found in OZIPM-4 is the variation in temperature during a simulation period. The chemical kinetic mechanism can be dependent on the variation of temperature. As the temperature rises, the kinetic mechanism generally reacts more rapidly, leading to earlier formation of ozone during the simulation period and possibly higher amounts of ozone. Temperature values are input in a manner similar to that in the MIXING option (described earlier and in Section 5). All temperature values must be in units of degrees Kelvin. If the TEMPERATURE option is not used, the default value is 303 K. Another constant temperature value may be set using the MECHANISM option card (see Table 8).

Surface Deposition

OZIPM-4 has the capability of treating dry deposition of gaseous species such as ozone, nitrogen dioxide, and sulfur dioxide. Hourly deposition velocities (in units of cm/s) are input for each species of interest. The format for surface deposition option (DEPOSITION) is the number of species with nonzero deposition rates followed by a series of lines that contain the species name and the first six hours of surface deposition rates. Additional hourly deposition rates are placed on lines following the first six hours of deposition rates. The user is referred to Section 5 for the format of the DEPOSITION option.

Initial Conditions of Transported Species

The TRANSPORT option is used to input initial concentrations of O_3, NMOC, and NO_2 transported in the surface layer and entrained from aloft. If the default mechanism is used, the concentrations of the transported species are entered on the first input line. If the user selects a different mechanism or wants to change the makeup of transported NMOC from the default value, the format for the NMOC inputs is different. Instead of entering the concentration for NMOC transported in the surface layer, a negative number is entered in that field on the TRANSPORT line. Similarly, a negative number is entered if there are organics entrained from aloft. These numbers must have absolute values equal to the number of organic species in the initial mix. Immediately following the TRANSPORT line, the concentration of NMOC transported in the surface layer and the fraction of the total organic for each organic species are input. Similarly, the concentration of NMOC aloft and the fraction of the total NMOC for each organic species are input on the third line of the transport option (or immediately following the TRANSPORT line if there is no surface transport of NMOC). Note that the fractions for the organic species in these two cases can differ. As is the case with all uses of the organic species, the fractions must be placed in the same order as the original list of names for the organic species input under the mechanism option. Ozone (surface and aloft) and NO_2 (surface and aloft) are input in the same manner regardless of the mechanism used.

To input species transported in the surface (or mixed) layer other than NMOC, O_3, and NO_2, an INITIAL option can be used. The number of transported species is placed on this line. The next line(s) contains a list of names of the species that are to have nonzero initial concentrations. (Up to 60 species may have nonzero initial concentrations.) The next line(s) contains the initial concentrations (ppm) of the species listed on the previous line(s). This INITIAL option is useful for continuing a calculation beyond the 24-hour limit of the model.

To consider entrainment of species other than NMOC, O_3, and NO_2, an ALOFT option can be used. The number of species with nonzero concentrations is placed on this line. The next line(s) contains a list of names of the species that are to have nonzero concentrations. (Up to 10 species may have nonzero initial concentrations.) The next line(s) contains concentrations (ppm) of the species listed on the previous line(s). These species will be entrained from aloft in a manner similar to that employed for ozone, NMOC, and NO_2, as previously described.

A set of background concentrations consisting of ozone, NMOC, and NO_2 can also be input by the user. The background concentrations represent the lowest limits that can be set for the transport concentrations in the surface and aloft layers. Therefore, if the user specifies values for O_3, NMOC, or NO_2 on the TRANSPORT line lower than the background values, the background values will be used. The format for the BACKGROUND option is similar to that for the TRANSPORT option except that only one set of values for O_3, NMOC, and NO_x is entered (see Section 5).

In general, the concentrations of species transported in the surface layer and aloft remain constant for any simulation on an isopleth diagram. The EKMA and the CREDIT options are the only options which allow the user to modify transported surface and aloft conditions for future year calculations.

Simulation Starting and Ending Times

Optional starting and ending times can be entered with the TIME option. The starting and ending times (local daylight time, based on the 24-hour clock) are placed in the second (Columns 11-20) and third (columns 21-30) ten-column fields, respectively. Times may be entered to the nearest minute, but the time difference (stop minus start) must not exceed 24 hours. Both the starting and ending times are set back to default values when a zero value is entered for the ending time.

Starting and ending times can also extend beyond midnight into the next day; the user need only specify the times. Note that the maximum of

24 hours for a simulation is not confined to a 24-hour period from midnight (0000 hr) to 2400 hours.

Emissions

There are three ways in which emissions can be input to OZIPM-4: the EMISSIONS, MASSEMISS, and MOLEMISS options. The MASSEMISS option allows the user to input VOC and NO_x emissions in units of kg/km^2 (Gipson, 1984). The hourly emission densities are converted to fractions of initial concentrations within the program based on the 0600 to 0900 measured NMOC and NO_x concentrations, and the initial mixing height (in meters). This procedure is described in the 1981 city-specific EKMA guidelines (EPA, 1981). The MOLEMISS option allows the user to input emissions of VOC, NO_x, and up to three other species (e.g., SO_2). Note that the user must input VOC and NO_x. The units of the hourly emissions values are in either ppm (ppmC for VOC) or moles (moles as carbon for VOC)/unit area. If moles/hr are input, the user must also input the initial mixing height and the horizontal area. The measured 0600 to 0900 NMOC and NO_x concentrations are required to convert VOC and NO_x molar emissions into emission fractions. The VOC and NO_x emissions will vary according to the initial NMOC and NO_x concentrations, whereas the emissions for the other species remain fixed and do not change with the 0600 to 0900 NMOC and NO_x concentrations.

As mentioned, up to five species may be input with the MOLEMISS option. The input species must be in the chemical kinetic mechanism (except for NO_x and VOC); otherwise, an error message will be printed. The nitrogen oxides emissions are input with the symbol NOX. The computer automatically splits NO_x into NO and NO_2, with a fixed NO/NO_x ratio of 0.95. Similarly, VOC emissions are input with the symbol VOC. The computer code will split the VOC emissions on the basis of the fractions input on the REACTIVITY line. The format for the MOLEMISS option requires the number of hours in which there are emissions (coded as a negative number), followed by the number of emission species. If units of moles are used, then the initial mixing height, followed by the horizontal area, is also added to the option line. Since post-0800 emissions are related to 0600-0900 measured ambient concentrations, 0600-0900 concentrations of VOC and NO_x, respectively, must be input in columns 51-60 and 61-70. The next line contains the 0600-0900 ambient concentrations of species other than VOC and NO_x with post-0800 emissions. The next line(s) will be the name vector for the emission species, followed by the emission values (6 on the first line; 7 on the second line; etc.) (See Section 5 for a more detailed description).

Reactivity of Initial Mix and VOC Emissions

Organic reactivity and the initial NO_2/NO_x ratio for both the 0600-0900 ambient mix and the VOC and NO_x emissions are input with the REACTIVITY line. This option must be used if the MECHANISM option is activated. The following entries must be made on the REACTIVITY line:

The number of organic species
The NO_2/NO_x ratio

If the number of organic species is nonzero, the next line(s) contains the vector describing the fractions of the total organic (per carbon basis) that each organic species represents. The order must be the same as that for the name and carbon number vectors entered earlier. The sum of the organic fractions should normally be equal to one. The default values for the organic fractions are set to the values recommended in Section 4, and apply only to the default CBM-IV mechanism.

OUTPUT OPTIONS

Output options are of two types:

(1) Perform a single simulation
(2) Estimate VOC control requirements

A single simulation is performed using the CALCULATE option. Two methods are available in OZIPM-4 for estimating VOC control requirements in compliance with the EPA guidelines (1981). The first method (ISOPLETH) requires the generation of at least one isopleth diagram in which all calculations are performed on the diagram. The second method (EKMA) is an automated version of the EPA guidelines that estimates the VOC control requirement based on inputs of base-case ozone and $NMOC/NO_x$ ratio into OZIPM. The first method has been described in detail by Whitten and Hogo (1978a) and Gipson (1984). The second method (originally implemented in OZIPM-2) is described by Gipson (1984). The EKMA option has been enhanced to handle the Appendix B guidelines (EPA, 1981) procedures regarding post-control levels of transported pollutants (Hogo and Whitten, 1985).

All three options are discussed in detail in the following section.

Performing a Single Simulation (CALC)

Individual simulations can be performed at specified initial NMOC and NO_x concentrations using the CALCULATE option. The first two numeric fields on the CALCULATE line (columns 11-20 and 21-30) specify the desired 0600-0900 ambient NMOC and NO_x concentrations. The initial conditions and hourly ozone concentrations will be printed to show the change of ozone with time during the simulation. Any number entered in the third numeric field (columns 31-40) will activate an information option that will print

The rate constants used in the kinetic mechanism,

The concentrations of all species in the kinetic mechanism,

The net rate of change of all species,

The reaction rates for each reaction, and

The photolysis constants for all photolysis reactions.

If the information option is activated, the user can then specify the simulation time (in minutes) for which concentrations of all species, current reaction rates, etc., will be printed. The number of minutes after the simulation starting time at which the initial printing is made (default value = 60 minutes after start) is entered in columns 41-50. The integral time step for which subsequent printings are made (default value = 60 minutes) is entered in columns 51-60. Under default values, hourly concentrations of species, net rates of change, etc., are printed. After the simulation has ended, a concentration versus time profile is printed for ozone. An example of output from this option is given in Section 6.

Calculating VOC Control Requirements for a Specific Case (EKMA)

A feature available in the OZIPM-4 program is the ability to perform a VOC emission reduction calculation without generating an ozone isopleth diagram. When the EKMA option is used, the user must supply information on the base-case ozone level to be reduced, the NMOC/NO_x ratio to be used in the calculation, and the percent change in NO_x emissions. The calculations are performed in accordance with the procedures used to calculate control estimates from an ozone isopleth diagram (EPA, 1981) Through an iterative search procedure, the base-case point is first located by finding the initial NMOC and NO_x concentrations (with the specified ratio) that produce the desired ozone concentration (within 0.005 ppm). A post-control point is then found by first adjusting the base-case NO_x point to reflect the change in NO_x emissions input by the user, and then finding the initial NMOC concentration that, along with the adjusted NO_x concentration, will produce an ozone value of 0.12 ppm (again, within 0.005 ppm). The VOC reduction estimate is then calculated as the percent change in NMOC concentration from the base-case point to the post-control point. The CREDIT option allows the user to specify changes in carbon monoxide emissions which may have an affect on VOC control requirements. The CREDIT option is used in conjunction with the EKMA option and is discussed in the following subsection.

Following Gipson (1984), the EKMA option is activated by an input record with the code word EKMA located in columns 1-4. The base-case ozone value is then placed in the first numeric field of the EKMA input record. The second numeric field of this record contains the NMOC/NO_x ratio. The percent change in NO_x emissions that is expected between the base case and the post-control time periods is coded in the third numeric field. This value should be entered as the percent change. Thus, a positive entry corresponds to an increase and a negative entry to a decrease. (For example, a 5 percent increase would be coded as 5.0, and a 5 percent decrease as -5.0.) The fourth numeric field is used to specify precursor transport conditions. If the concentration of transported NMOC, O_3, and NO_x is assumed to be zero for the post-control case, this entry may be left blank. Otherwise, a numeric entry (e.g., 1.0) denotes that non-zero transport conditions are used for the post-control case and these values are coded in the next input record.

The first two fields of this next input record contain the future surface and aloft ozone concentrations (in ppm), respectively. If a negative value is input, then future-year ozone transport is estimated using the curves described in EPA (1987) and shown in Figure 4. The third field contains the concentration of NMOC transported in the surface layer for the post-control situation. A negative value represents the median NMOC contribution factor as described in Appendix B of the 1981 guidelines (EPA, 1981). The fourth field represents the concentration of NMOC transported aloft for post-control conditions. A negative value represents a 40 percent reduction in present-day NMOC aloft. The next two fields (five and six) contain the future NO_x surface and aloft transport levels (in ppm). The user should note that the structure of this input record is similar to that of the TRANSPORT input record in that if any entry is left blank, then the transport level for that species will be set to zero for the post-control case. Also, no provisions are included for making any changes in the composition of NMOC used in the simulations (i.e., the same NMOC transport composition will be used for both base case and post-control point).

The last line of the EKMA option contains the measured 0600-0900 NMOC and NO_x values, which are used internally by OZIPM-4, if necessary, to determine the location of the base-year ozone should it occur more than once along the NMOC/NO_x line (i.e., the occurrence of a maximum along the NMOC/NO_x line). This line is also used to input the base-year NMOC and NO_x concentrations (in units of ppmC and ppm) in columns 21-30 and 31-40 if the user already has this information from single CALC runs or from previous simulations. If a negative NMOC/NO_x ratio has been entered on line 1 of the EKMA option, OZIPM-4 will read the base-year NMOC and NO_x values and skip to the future-year control estimates. This capability

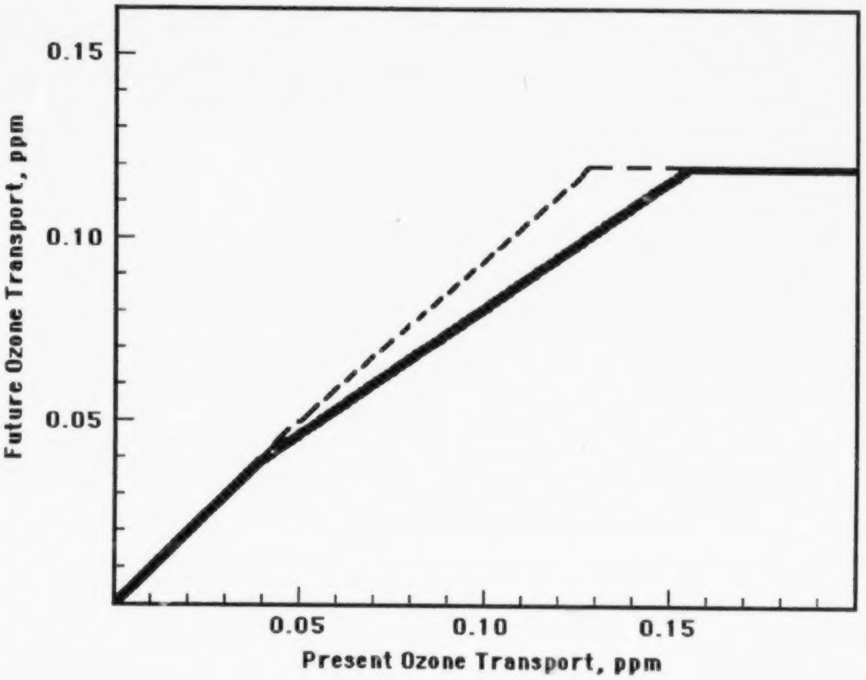

FIGURE 4. Future ozone transport as a function of present transport.

saves computer time and costs. The last field (five) of this record allows the user to calculate peak O_3 for a given percent reduction in NMOC.

As just described, the EKMA option causes the program to compute the VOC reduction (in percent) needed to lower the base ozone to 0.12 ppm. Another option available to the user is the ability to generate supplemental information. An entry of 1.0 in the fifth numeric field of the EKMA line generates a tabular report showing the change in ozone as a function of percent change in VOC. Predicted ozone corresponding to VOC reductions of 10 percent, 20 percent, 30 percent, ..., and 100 percent, respectively, are printed. If a value of 2.0 is coded instead, the predicted ozone concentrations will also be written to a user-defined file, which might be used for subsequent analysis or graphical display. One output record is written to the file for each EKMA option that is activated. The output format consists of 11 fields, each 5 columns wide. The first field (columns 1-5) contains the base-case ozone value. The remaining 10 fields contain the ozone predictions corresponding to the VOC reductions of 10 percent, 20 percent, 30 percent, ... 100 percent, in that order. The user can perform a single specified VOC reduction if a nonzero value is declared in the sixth numeric field.

Carbon Monoxide (CO) Emission Credits

As part of the development of the CBM-IV mechanism it was discovered that elevated concentration levels of carbon monoxide (CO) may have an affect on the resultant VOC control requirement. Levels of CO typically around 1.2 ppm in the surface layer are observed in many parts of the U.S. This level of CO may have significant contributions to the ozone formation process. Based on historic trends in CO emissions and ambient concentrations of CO (Baugues, 1987), it was determined that reductions in CO emissions can account for part of the reductions in ambient ozone levels. Based on these analyses, the U.S. EPA is allowing credits for CO emission reductions in determining VOC control requirements. This "credit" allowance is handled within the OZIPM-4 computer program through the use of the CREDIT option.

The CREDIT option is currently used for CO emissions only. The first line containing the CREDIT option contains the number of hours of post-0800 CO emissions fractions (columns 21-30). A negative value is used when mass emissions of CO (in units of kg/km^2) are input. The initial mixing height is entered in columns 31-40. The next line contains the measured 0600-0900 CO concentration, present and future year CO concentrations transported aloft, and the percent change in CO emissions. If the user inputs a 0600-0900 present-day CO concentration in columns 11-20, that value will be reduced in the future-year calculations by the percent change in CO emissions that is entered in columns 41-50. The following line contains either the hourly emission fractions or mass emissions of CO. The input formats for the CREDIT option is described in Section 5.

If the CREDIT option is not invoked, CO concentrations are defaulted to 1.2 ppm for the 0600 to 0900 concentration and 0.5 ppm aloft with no change in future year levels.

Generating an Isopleth Diagram (ISOP)

Up to six options can be used when generating an isopleth diagram: ISOPLETH, TITLE, PLOT, SPECIES, ACCURACY, and ALREADY. These options are described next.

ISOPLETH Option

In all OZIPM-4 isopleth diagrams, the origin represents 0.0 initial 0600-0900 NMOC concentrations (ppmC) and 0.0 NO_x concentrations. The maximum NMOC and NO_x values represented on the abscissa and the ordinate can be changed from their respective default values of 2.0 ppmC NMOC and 0.14 ppm NO_x by inputting the desired maxima into the first two numeric fields of the ISOPLETH line. The desired maximum NMOC concentration should be placed in the field of columns 11 through 20. The desired maximum NO_x concentration should be placed in the field of columns 21 through 30.

Any number can be used for the desired maximum NMOC and NO_x concentrations; however, because the scales on the abscissa and the ordinate are divided into ten and seven divisions, respectively, only certain values of the maxima will produce even markers. Thus, to produce an easy-to-use diagram, the NO_x maxima should be evenly divisible by seven (e.g., 0.14, 0.21, 0.28, 0.35, etc.). Similar consideration should be given to selecting an NMOC maximum.

The desired number of isopleths in the diagram should be inserted (followed by a decimal point) in the field of columns 31 through 40 of the ISOPLETH line. Up to 20 isopleths can be drawn (the default value is 11). OZIPM-4 then reads the proper number of fields from the succeeding line or lines to provide the ozone concentrations (in units of ppm) for which isopleths are to be drawn. For example, inserting 10.0 in columns 31-34 of ISOPLETH causes OZIPM-4 to read the seven 10-space numeric fields on the next line and three on the succeeding line. (As noted earlier, OZIPM-4 does not read past column 70 on any line except the program title line.)

OZIPM-4 can provide isopleth diagrams for up to five species when the SPECIES option is specified. The user must enter the number of species to be plotted in columns 61 to 70. The program will read the appropriate sets of isolines to be plotted based on the value in columns 61 to 70 (one set per species). The number of isolines for each set is determined from the value entered in columns 31 to 40. The user enters the values for each set of isoline after the ISOPLETH line.

TITLE Option

The title can be changed by inserting a line with the word TITLE followed by a line with the desired title. Everything in columns 1 through 72 of this title line will be printed on the output and isopleth diagrams in place of the default title, "Standard Ozone Isopleth Conditions." As with all options, these lines must precede the ISOPLETH or CALCULATE options.

PLOT Option

Any plotting package that can be called using the standard CALCOMP subroutines can be used. Calls to these routines are activated by a line with the code word PLOT. This line must precede the ISOPLETH option. The actual CALCOMP routines called are PLOTS, PLOT, NUMBER, SYMBOL, and NEWPEN (if necessary). The use of the CALCOMP routines is discussed in Section 5.

The user also has the option to specify the actual size of the plot by defining the lengths (in inches) of the sides of the diagram. Columns 31-40 are used for the abscissa of the diagram. Columns 41-50 are used for the ordinate of the diagram. The size of title characters and axes numbers and the size of the isopleth labels can also be set by the user in columns 51-60 and 61-70, respectively. The default values are given in Section 5. If the user wishes to reset any of these values, it is recommended that all values change proportionally.

Another option on the CALCOMP plots is the overlay of gridded lines on the isopleth diagram. This is done by declaring any nonzero positive values in columns 21-30. If this option is exercised, a grid of different colors will be overlaid onto the diagram. If the user does not have access to the choice of different pen colors, use of this option is not recommended. If there is access to a matrix plotter (such as the VERSATEC plotter) and the choice of lines consists of thickness and pattern (i.e., dot-dash on solid patterns) the user can then enter a negative nonzero value in columns 21-30. The absolute value of the number entered represents the user's choice of pattern and thickness. This number varies with different computer systems.

SPECIES Option

The OZIPM-4 package also has the capability of plotting an isopleth for any species in the kinetic mechanism. For instance, a user may be interested in plotting NO_2 or PAN (peroxyacetylnitrate) isopleths. To activate this option, the user inputs a line with the word SPECIES in the first 10-column field and the number of species to be plotted. On the next line, the species names (or alphanumeric symbols), as used in the kinetic mechanism, are placed in the first four columns of each 10-column field (i.e., 1-4, 11-14, 21-24). The program will calculate maximum one-hour values for the species of interest. Isopleth diagrams will be generated for all species of interest when the ISOPLETH option is used, as noted earlier. If the SPECIES option is not used, the program will be set to the default species O_3 (ozone). The SPECIES option can also be used with the CALCULATE option to generate concentration-time plots for the species of interest.

ALREADY Option

When constructing isopleth diagrams, results from previous simulations can be utilized with the ALREADY option. To incorporate results from a previous run, the following conditions must be identical in both runs: the NMOC and NO_x scales and the city-specific options. Such a situation could occur when

An initial run is terminated because of a time restriction;

The user wishes to repeat the run with the PLOT option to obtain a CALCOMP-generated plot;

The user wishes to alter the tension factors used in the interpolation schemes; or,

The user wishes to plot an isopleth for a species using a different set of isolines.

To input the results of previous runs, the number of completed simulations is entered in the first numeric field (columns 11-20) of the ALREADY line. The results of those simulations must be entered on the following lines in the same order in which they are calculated. Each line contains the results of one simulation. Field 1 (columns 1-10) contains the initial NMOC concentration, field 2 (columns 11-20) contains the initial NO_x concentration, and field 3 (columns 21-30) contains the resulting maximum one-hour average O_3 (or other species) concentration. If a negative number of completed simulations is entered, then OZIPM-4 will read the completed simulation results from an external file automatically generated by the OZIPM-4 from the previous run.

ACCURACY Option

The ACCURACY option controls the precision of numerical schemes used in generating an isopleth diagram. The OZIPM-4 performs 121 simulations. The spline tension factors used for the spline interpolation routines are specified in columns 41-50 and 51-60. Since the ISOPLETH option requires greater amounts of execution time, the user is advised to perform several single calculations near the maximum NMOC and NO_x concentrations to assure that the base-case ozone isoline occurs near the upper right portion of the diagram. Poor choices for the maximum NMOC and NO_x concentrations can lead to isolines occurring off the diagram or may be compressed into a small part of the diagram.

A considerable amount of computer time is wasted when the maximum one-hour average O_3 concentration in a simulation occurs early but the simulation is continued for the full simulation period. The default condition in OZIPM forces this continuation because two ozone peaks could occur in simulations, and the second may be the larger. Nevertheless, a sizable reduction in computer costs is possible for simulations with single ozone peaks if the simulations are stopped after their peaks are reached. This can be done in OZIPM-4 by placing any number in the sixth numeric field (columns 61-70) of the ACCURACY line. However, the reasons for the occurrence of two ozone peaks are not well underdstood, so the full simulation period must be used to generate isopleth diagrams intended for control strategy use.

Testing the Accuracy of the Isopleth Diagram

Options have been incorporated into OZIPM-4 that allow users to test the accuracy of the diagram. In this manual, the term "accuracy" is always used in reference to the numerical solution of an implied initial value problem in ordinary differential equations. Thus, accuracy does not refer to the degree of correspondence between an isopleth diagram and atmospheric data.

Although the experience gained in the development of OZIPM-4 suggests that the default number of simulations, tension factor, and so on, will generate sufficiently accurate isopleth diagrams, this experience does not guarantee sufficient accuracy. Recommended procedures for checking many of the factors that affect accuracy are all similar. They merely answer the following question: Do somewhat higher or somewhat lower values of a particular factor significantly affect the resulting isopleth diagram? OZIPM-4 has been designed to respond properly to these factors. The procedures used in OZIPM-4 to check accuracy and to generate additional information are discussed next.

(1) Accuracy of Simulations. The numerical integration scheme employed in OZIPM-4 estimates the degree of error at every step of the integration. The size of the time step taken by the computer is adjusted to keep the estimated error in the specified range. The error is conveniently controlled by a single parameter with a default value of 0.003. Smaller values of this parameter increase both the accuracy and computer time. Larger values do the opposite. By entering numbers smaller than 0.003 in the third numeric field of the ACCURACY option line (columns 31-40), one can estimate the accuracy of the simulations. For example, if several CALCULATE and ACCURACY lines are used, several simulations can be performed using the same NMOC and NO_x concentration, but using different time steps in the numerical integration. This procedure can be used to demonstrate how the simulation results vary with increased error tolerance.

(2) Spline Interpolation Accuracy. Unfortunately, the spline functions used to interpolate between simulation results do not have a parameter as relevant to accuracy as does the numerical integration scheme used for the simulations. The spline functions can be controlled to a limited extent by a simple factor that is analogous to tension. The lowest values for this factor (e.g., 0.001) cause the hyperbolic spline function to resemble cubic splines, whereas the high values (e.g., 50.0) result in virtually straight lines between points (or simply linear interpolation). Interpolation occurs in two different stages of OZIPM-4 and two factors are available to control tension. The first factor controls the first stage, namely interpolation between diagram points along a line of constant $NMOC/NO_x$ when the EKMA option is invoked. This interpolation stage estimates the coordinates of ozone concentrations when a maximum occurs along the line of constant $NMOC/NO_x$.

The second factor controls the interpolation between diagram points calculated in the ISOPLETH option to generate the coordinates of the isopleths themselves. Default values for both are 1.0, and the user can change these factors by entering the desired number in the fourth and/or fifth numeric field of the ACCURACY option line (columns 41-50 and 51-60). Thus, a value of 50.0 in the fourth numeric field of the ACCURACY line would cause nearly linear interpolation to be used to locate the points on the line of constant NMOC/NO_x that correspond to the ozone concentrations to perform the EKMA option. A value of 50.0 in the fifth field would result in nearly straight lines between diagram points calculated.

SECTION 4

USING THE CBM-IV IN OZIPM-4

This section presents a description of the CBM-IV and guidance for its use in OZIPM-4. The Carbon-Bond concept (Whitten, Killus, and Hogo, 1980) was developed mainly to simplify chemical kinetics mechanism use in atmospheric applications. Therefore, the simple procedures developed for earlier versions of the Carbon-Bond Mechanism used in EKMA and published in several documents can, for the most part, be applied to the use of the CBM-IV. The most recent documentation for using Carbon-Bond chemistry in EKMA can be found in Hogo and Whitten (1985), Killus and Whitten (1984), and Gipson (1984). The detailed development of the CBM-IV is documented in Gery, Whitten, and Killus (1988). This mechanism is actually a hybrid of explicit chemistry, surrogate approximations, and lumped/generalized chemistry designed to simulate the broad features of urban smog chemistry. Explicit chemistry is used to treat the inorganic and carbonyl species plus the chemistries of ethene, toluene, and xylene. The carbon-bond lumping method is used primarily for paraffins and olefins.

Each part of the CBM-IV chemistry, such as the inorganic subset or the ethene chemistry, conforms to current literature review studies and has been extensively tested against smog chamber data on organics/NO_x systems, including complex mixtures intended as surrogates for urban air samples. In addition, the entire CBM-IV was used to simulate a series of auto exhaust and synthetic auto exhaust experiments involving a variety of conditions. Most of the smog chamber experiments used for CBM-IV testing were performed in the outdoor dual-chamber facility of the University of North Carolina, which is a well-characterized chamber with extensive analytical capabilities. The CBM-IV has also been tested with experimental data from chambers at the University of California at Riverside and Battelle Columbus Laboratories.

DEFAULT CBM-IV MECHANISM

The default chemical mechanism implemented in OZIPM-4 is the CBM-IV mechanism presented in Appendix A. The CBM-IV mechanism consists of 34 chemical species and 82 chemical reactions. The CBM-IV contains 9 primary organic species (see Table 1).

TABLE 1. Carbon Numbers of Carbon-Bond Groups for Primary Species

Carbon-Bond Group	Carbon Number (carbon atoms per molecule)
PAR	1
ETH	2
OLE	2
TOL	7
XYL	8
FORM	1
ALD2	2
ISOP	5
NR	1

The species NR represents the nonreactive part of different molecular species such as benzene, ethane, and acetylene. The concentrations of several species whose concentrations do not vary (such as O_2 and N_2) are lumped in with the rate constant. Unless a different value is entered by the user, the concentration of H_2O used in the CBM-IV corresponds to 50 percent relative humidity (20,000 ppm) at approximately 303 K. It is not recommended that this value be changed by the user. However, if desired, a different H_2O concentration can be entered using the INIT option.

The CBM-IV mechanism shown in Appendix A is that discussed by Gery, Killus, and Whitten (1988) except that one reaction has been added. That reaction is:

$$NR \rightarrow NR \qquad k = 1\ \text{min}^{-1} ,$$

which is added to account for the nonreactive species.

DEFAULT PHOTOLYSIS RATE CONSTANTS

The CBM-IV chemical mechanism contains 11 photolysis reactions that vary with solar zenith angle (see Table 2). The photolytic rate constants for NO_2 are stored in OZIPM-4 as a function of zenith angle. These rates, which were derived by Jeffries and Sexton (1987) and Gery, et al. (1988),

TABLE 2. CBM-IV Photolysis Reactions.

Reaction Number	Multiplication Reaction	Photolysis Rate
1	$NO_2 + h\nu \rightarrow NO + O$	See Table 3
8	$O_3 + h\nu \rightarrow O(^3P)$	0.053 x k_1*
9	$O_3 + h\nu \rightarrow O(^1D)$	See Table 4
14	$NO_3 + h\nu \rightarrow 0.89\ NO_2 + 0.89\ O(^3P) + 0.11\ NO$	33.9 x k_1*
23	$HNO_2 + h\nu \rightarrow NO + OH$	0.1975 x k_1*
34	$H_2O_2 + h\nu \rightarrow 2OH$	0.189 x k_{39}*
38	$FORM + h\nu \rightarrow 2HO_2 + CO$	See Table 4
39	$FORM + h\nu \rightarrow CO$	See Table 4
45	$ALD2 + h\nu \rightarrow XO_2 + 2HO_2 + CO + FORM$	See Table 4
69	$OPEN + h\nu \rightarrow C_2O_3 + HO_2 + CO$	8.40 x k_{38}*
74	$MGLY + h\nu \rightarrow C_2O_3 + HO_2 + CO$	8.96 x k_{38}*

* Photolysis rate factors for ratioing to the recommended NO_2 (Table 3) HCHO (Table 4) rates must be recalculated if NO_2 and HCHO rates other than the recommended values (Jeffries and Sexton; 1987) are used. That is, new ratios may have to be calculated for these species if the reference rate is changed.

are the recommended j-values and are given in Table 3. The default values represent the reaction rate constants at approximately 640 m above sea level (which are more representative of the entire mixed layer).

Three of the photolysis reactions shown in Table 2 (Reactions 8, 14, and 23) vary with zenith angle in a manner similar to that of NO_2 photolysis. The photolytic rate constants for these reactions can be described by applying a single multiplication factor to the NO_2 photolytic constants. (For example, the multiplication factor for Reaction 9 is 0.053.) The multiplication factor is input into the rate constant slot of the reaction line as described in the MECHANISM option in Section 5.

Seven of the reactions in Table 2 have photolysis rates that vary with zenith angle independent of NO_2 photolysis. The default ratios to NO_2 potolysis for four of these reactions (Reactions 9, 38, 39, and 45) are stored in OZIPM-4 and are shown in Table 4. As described in Section 5, a multiplication factor of 1.0 is entered into the rate constant slot of the reaction line for these reactions.

Two of the species shown in Table 2 (OPEN and MGLY) are expected to photolyze with a zenith-angle dependence similar to that of formaldehyde photolysis to radicals (Reaction 38); H_2O_2 has a zenith-angle dependency that is similar to the photolysis of formaldehyde to stable products (Reaction 39). We therefore use the zenith-angle-dependent ratios given in Table 4 as default values for these reactions and multiply the resulting rates by the factors given in Table 2. If new rates other than those recommended in Table 4 are used, the factors given in Table 2 may have to be recalculated to maintain the same absolute rate constant.

DEFAULT VOC AND NMOC REACTIVITIES

Table 5 lists the default carbon fractions associated with NMOC transported in the surface layer and entrained from aloft. These values were determined by Jeffries, Sexton, and Arnold (1987) through analysis of data from aircraft samples collected above the morning inversion layer over four urban areas. Jeffries, Sexton, and Arnold (1987) also analyzed data from more than 800 ground-level samples collected between 0800-0900 in a large number of urban areas to derive default reactivities for the initial NMOC and VOC emissions. These default carbon fractions are given in Table 6.

The reactivity resulting from global background concentrations of methane is represented by Reaction 51 in the CBM-IV, where an average background level of 1.85 ppm is assumed for methane. The effect of carbon monoxide on urban O_3 formation is represented by Reaction 36 in the CBM-IV. CO concentration levels are defaulted to 1.2 ppm CO for the 0600 to

TABLE 3. NO_2 Photolysis Rate Constants Stored in OZIPM-4. (Source: Jeffries and Sexton, 1987)

Zenith Angle	Rate Constant*
0	0.5893
10	0.5851
20	0.5713
30	0.5470
40	0.5093
50	0.4537
60	0.3740
70	0.2578
78	0.1341
86	0.0242

* Units are min^{-1}.

TABLE 4. Photolysis Reaction Rate Ratios Stored in the OZIPM-4.* (Source: Jeffries and Sexton, 1987)

Zenith Angle	ALD2 + $h\nu \rightarrow XO_2$ + 2HO2 + CO + FORM	FORM + $h\nu \rightarrow$ CO‡	FORM + $h\nu \rightarrow$ 2HO2 + CO§	$O_3 + h\nu \rightarrow O(^1D)$
0	5.89E-4	5.75E-3	3.70E-3	4.61E-3
10	5.78E-4	5.73E-3	3.66E-3	4.48E-3
20	5.50E-4	5.67E-3	3.56E-3	4.13E-3
30	5.03E-4	5.54E-3	3.40E-3	3.59E-3
40	4.36E-4	5.35E-3	3.14E-3	2.87E-3
50	3.55E-4	5.08E-3	2.80E-3	2.08E-3
60	2.57E-4	4.63E-3	2.33E-3	1.24E-3
70	1.59E-4	4.01E-3	1.74E-3	5.43E-4
78	8.95E-5	3.48E-3	1.28E-3	2.24E-4
86	8.26E-5	5.25E-3	1.78E-3	1.24E-4

* Ratios are relative to NO_2 photolysis. Rate constants are determined by multiplying the ratio by k_{NO_2}.

‡ These ratios, multiplied by the factor in Table 2, are also used for H_2O_2.

§ These ratios, multiplied by the factors in Table 2, are also used for MGLY and OPEN.

TABLE 5. Carbon Fractions for Transported NMOC (Source: Jeffries, Sexton, and Arnold, 1987).

Species	Fraction*
ETH	0.034
OLE	0.020
ALD2	0.037
FORM	0.070
TOL	0.042
XYL	0.026
PAR	0.498
ISOP	0.00
NR	0.273

* Applies to NMOC transported in the surface layer and entrained from aloft.

TABLE 6. Reactivity of Initial Mixture and VOC Emissions. (Source: Jeffries, Sexton, and Arnold, 1987)

Bond Type	Default Value
ETH	0.037
OLE	0.035
ALD2	0.052*
FORM	0.021*
TOL	0.089
XYL	0.117
PAR	0.564
ISOP	0.00
NR	0.085

* Estimated.

0900 concentration and 0.5 ppm CO entrained from aloft unless the user explicitly specifies other concentration levels using either the INITIAL or CREDIT options.

SELECTING A USER-SPECIFIED ORGANIC REACTIVITY

Ambient organic measurements are not routinely collected due to the intensive efforts required to collect the data. However, if 0600-0900 ambient organic measurements are available, they should be used to calculate organic reactivity rather than using the default carbon fractions that are stored in OZIPM-4. Table 7 shows how to determine the CBM-IV fractions from 0600-0900 ambient data reported in moles/ℓ.

The following paragraphs describe step-by-step how the organic reactivity is defined based on the ambient measurements shown in Table 7. Before we discuss these procedures, we note that in general ambient measurements are reported in the following units:

ppm (parts per million)
pphm (parts per hundred million)
ppb (parts per billion)
$\mu g/m^3$ (micrograms per cubic meter)

In some cases the organic compounds may be expressed in the above units either as a molecular total or as a carbon total (i.e., the actual molecular weight or the molecular weight of carbon is used). In general, chemical mechanisms are based on molecular reactions or the number of molecules involved. The first three units presented above are in the units necessary for most chemical mechanisms. The fourth unit is a mass unit and must be converted to molecular units. The following equation is used to convert mass units to molecular units:

$$C_{ppm} = \frac{0.0244}{MW} \times C_{\mu g/m^3} \quad ,$$

where MW is the molecular weight in units of g/moles of the organic compound. Molecular weights for many compounds are given in Table B-1. The conversion factor, 0.0244, is based on the perfect gas law at 25°C and standard pressure. To obtain molecular units as carbon, one needs to multiply by the number of carbons found in the organic compound.

Table 7 shows ambient organic compound measurements in the Los Angeles area (Calvert, 1976). The measurements are reported in molar units (ppm in this case); to obtain the carbon-bond reactivity, one must

TABLE 7. Carbon-bond splits for Los Angeles ambient measurements.*

(a) Carbon-Bond Group Concentrations

Compound	[RH], ppm Molar Basis	Number of Each Bond Group x Concentration							
		NR	OLE	ETH	PAR	FORM	ALD2	TOL	XYL
CH_4	2.01								
C_2H_6	0.049	0.078			0.020				
C_2H_4	0.043			0.043					
C_2H_2	0.038	0.038			0.038				
C_3H_8	0.037	0.056			0.056				
C_3H_6	0.0087		0.0087		0.0087				
iso-C_4H_{10}	0.012				0.048				
n-C_4H_{10}	0.037				0.148				
1-C_4H_8	0.0015		0.0015		0.0030				
iso-C_4H_8	0.0030				0.009	0.003			
iso-C_5H_{12}	0.0443				0.2215				
n-C_5H_{12}	0.0162				0.0810				
Cyclo-C_5H_{10}	0.0026				0.013				
1-C_5H_{10}	0.004		0.004		0.012				
2-Methylbutene	0.0008				0.0024		0.0008		
2,3-Dimenthylbutane**	0.0008				0.0048				
2-Methylpentane	0.0110				0.0660				
3-Methylpentane	0.0100				0.0600				
1-Hexene	0.0017		0.0017		0.0068				
n-Hexane	0.0100				0.0600				
Cyclohexane***	0.0107				0.0642				
2,2,3-Trimethylbutane	0.0077				0.0539				
C_6H_6	0.0082	0.041			0.0082				
2-Methylhexane	0.0069				0.0483				
3-Methylhexane	0.0063				0.0441				

Continued

* Source of hydrocarbon data: Calvert (1976).
** Incorrectly reported as 2,2 dimethylbutene by Calvert (1976).
*** Incorrectly reported as cyclohexene by Calvert (1976).

TABLE 7. Concluded.

Compound	[RH], ppm Molar Basis	Number of Each Bond Group x Concentration							
		NR	OLE	ETH	PAR	FORM	ALD2	TOL	XYL
1-Heptene	0.0044		0.0044		0.0220				
n-C_7H_{16}	0.0043				0.0301				
Methylcyclohexane	0.0037				0.0259				
2,2,3- and 2,3,3-Trimethylpentane	0.0019				0.0152				
2,2,4-Trimethylpentane	0.0025				0.0200				
Toluene	0.020							0.020	
1-Methylcyclohexene	0.0047		0.0047		0.0235				
2,2,5-Trimethylhexane	0.0010				0.0090				
n-C_8H_{18}	0.0021				0.0168				
EtC_6H_5	0.0041				0.0041			0.0041	
p,m-Xylenes	0.0140								0.0140
o-Xylene	0.0060								0.0060
n-C_9H_{20}	0.0013				0.0117				
n-PrC_6H_5	0.0010				0.0020			0.0010	
sec-BuC_6H_5	0.0050				0.0150			0.0050	
n-$C_{10}H_{22}$	0.0011				0.0110				
n-$C_{11}H_{24}$	0.0010				0.0110				
n-$C_{12}H_{26}$	0.0003				0.0036				
CO	1.91								
Total		0.213	0.025	0.043	1.2978	0.003	0.0008	0.0301	0.0200

(b) Carbon-Bond Splits

Compound	NMHC (ppm)	ppmC	Carbon Fraction of NMHC*	Adjusted Carbon Fraction*
NR	0.213	0.213	0.099	0.099
ETH	0.043	0.086	0.040	0.040
PAR	1.298	1.298	0.603	0.603
FORM	0.025	0.025	0.012	0.032
OLE	0.025	0.050	0.023	0.023
ALD2	0.0008	0.0016	0.001	0.036
TOL	0.030	0.210	0.098	0.098
XYL	0.020	0.160	0.074	0.074
Total		2.044	0.950	1.000

* Carbon fractions adjusted to account for an estimated 5 percent fraction of unmeasured aldehydes.

assign the individual carbon atoms of each organic compound to the appropriate carbon-bond group according to Table B-2 in Appendix B. Table B-2 shows the breakdown of each carbon atom from the molecular compound to the carbon-bond groups. For example, the organic compound C_3H_6 (propylene) shown in Table 7 comprises one OLE and one PAR. Thus, of the three carbon atoms of propylene, two are assigned to OLE (because each OLE group contains two carbons), and one is assigned to PAR. To calculate the concentrations of OLE and PAR from propylene, we multiply the number of each bond group by the concentration of propylene. Thus, the propylene concentration of 0.0087 ppm produces 0.0087 ppm of OLE and 0.0087 ppm of PAR. As another example, Appendix B shows that benzene (C_6H_6) consists of five NR and one PAR. Applying the above procedures, we obtain 0.041 ppm of NR and 0.0082 ppm PAR.

This procedure is followed for all the organic compounds identified in Table 7. The carbon-bond concentrations are summed as shown in Table 7(b). The OZIPM-4 requires all organic fractions to be on a "per-carbon" basis. Thus, the concentrations for each carbon-bond group are multiplied by the appropriate number of carbons reported in Table 1 and normalized to obtain the carbon fractions, as shown in the fourth column of Table 7(b).

In the example presented in this section, only surrogate carbonyls could be included in the speciations because carbonyl compounds per se (aldehydes and ketones) could not be detected by the instrumentation used. Carbonyl compounds were undeniably present, however, and they are significant contributors to smog chemistry. Therefore, some estimates of carbonyl emissions must be made. Investigations by Killus and Whitten (1984) show that an estimated 5 percent of the total organics can be carbonyls. Of the 5 percent, 60 percent is assumed to be ALD2, and 40 percent is assumed to be FORM. Thus, for those cases in which there are no measured carbonyls, we must add 5 percent carbonyls (3 percent ALD2 and 2 percent FORM) to the total organics. The carbon fractions adjusted for the carbonyls are shown in the fifth column of Table 7(b). The numbers shown in this column would be entered into the OZIPM-4 program.

An alternative method for comparing calculated carbon fractions is to estimate an average K_{OH} value. K_{OH} values are rate constants that provide the per-carbon measure of the reactivity of a class of compounds with OH radicals. The weighted sum of the K_{OH} value for each individual NMOC species can provide an estimate of the overall reactivity of the NMOC. Using the CBM-IV species rate constants with OH radicals (see Appendix A), we can describe an average K_{OH} as

$$K_{OH} = \mathrm{PAR} \times 1203 + \mathrm{ETH} \times 5824 + \mathrm{OLE} \times 20422 + \mathrm{ALD2} \times 11833 + \mathrm{TOL} \times 1284 + \mathrm{XYL} \times 4497 + \mathrm{FORM} \times 15000.$$

where the numbers represent the per-carbon reaction rate with OH for each CBM-IV at 303 K.

Average K_{OH} values should fall between 2700 and 3600 min^{-1} (Baugues, 1987). Thus, on the basis of the calculation presented in Table 7 and the foregoing equation, the calculated K_{OH} is about 2835 min^{-1}, which is within the recommended range.

SECTION 5

USER'S GUIDE

This chapter describes the format of the input data, the types of errors and warning messages that can occur, and some special problems to be considered in the installation of the program on a specific facility.

FORMAT OF INPUT DATA

The 26 options in OZIPM-4, which were discussed in Section 3, are listed in Table 8.* For each option, the locations of the different parameters on the appropriate lines are shown. The order of the OZIPM-4 options in the input file is not important except for the ISOPLETH, EKMA, and CALCULATE options. Any options to be activated for simulations must precede these three options. Consequently, the order shown in Table 8 is recommended. This ordering has the MECHANISM and ZENITH options listed first, followed by the options used to input city-specific information (PLACE, DILUTION, EMISSIONS, REACTIVITY, TRANSPORT, CREDIT, etc.). The next group of options affects some of the operational aspects of OZIPM (ACCURACY, ALREADY, PLOT, SPECIES, and TIME). The options that actually initiate simulations follow (CALCULATE EKMA, and ISOPLETH). The last line of any input set must be a blank line.

As shown in Table 8, all four-letter code words (e.g., TITL, PLAC, etc.) that activate an option must begin in column 1. Each data line containing such a code word has up to six numeric fields, each ten spaces wide, beginning in column 11. An entry can be made anywhere in a field, but a decimal point must always be used, even with integral values. Additional data lines are associated with some options. These lines must follow the option line in the order specified in Table 8. For example, the line containing the title must immediately follow the line with the code word TITL. Data lines that do not begin with code words can contain up to seven 10-column fields beginning in column 1. Similar to the numeric fields on lines with code words, entries may be made anywhere in the field provided a decimal is used.

---

* For convenience, Table 8 appears at the end of this section.

As previously described, most parameters have associated default values. These are indicated by DF in Table 8. If no entry is made in a numeric field, the default value will be assumed. For example, if the only entry made on the PLACE option line is in the first numeric field, the default value of 118.25 will be assumed for the second numeric field, 8.0 for the third, etc.

PROGRAM-GENERATED ERROR MESSAGES

This section discusses potential output error messages produced by OZIPM. Two types of error messages can be generated:

(1) Fatal error messages--messages caused by problems that immediately halt any further computation.

(2) Nonfatal error messages--messages caused by problems that do not cause an immediate halt in computation.

These types of messages are discussed next.

Fatal Error Messages

Seven fatal error messages can occur during OZIPM-4 runs. Five of these occur because the integration scheme cannot proceed further. The following error messages all stem from problems encountered in the integration scheme routines:

```
PROBLEM APPEARS UNSOLVABLE WITH GIVEN INPUT

INTEGRATION HALTED BY DRIVER AT T - ____, EPS TOO SMALL TO BE
ATTAINED FOR THE MACHINE PRECISION

KFLAG = -2 FROM INTEGRATOR AT T = ______, H = ______ THE REQUESTED
ERROR IS SMALLER THAN CAN BE HANDLED

KFLAG = -3 FROM INTEGRATOR AT T = _____ CORRECTOR CONVERGENCE COULD
NOT BE ACHIEVED

ILLEGAL INPUT..EPS.LE.0
```

If any of these messages occur, the user should try the following procedures:

Check input to be sure all data are correct (e.g., check NMOC and NO_x values on a CALCULATE option, check for negative error tolerance, and so on).

Raise the value of the error tolerance (ACCURACY option), if necessary.

As a last resort, alter the simulation conditions slightly (e.g., change emissions, dilution, etc.).

Nonfatal Error Messages

One nonfatal error message can occur in OZIPM-4 runs. The user may wish to redefine the situation (i.e., the limits of the diagram) or to check the input data.

THE OPTIONS INSTRUCTION___CANNOT BE PROCESSED

If this message occurs, the user should check for an error in the input data.

COMPUTER CONSIDERATIONS

The OZIPM program consists of one main program and 55 subprograms. It requires about 30,000 16-BIT words of core in a PRIME 750 computer system. Run times on the system average 30 minutes for an isopleth plot and around 3 minutes for an EKMA calculation. A complete listings of the OZIPM-4 code is shown in Volume 2. Also included are five calls to CALCOMP subroutines. The following paragraphs discuss special language considerations, use of CALCOMP routines, and computer control language.

Language Considerations

Although OZIPM-4 has been written to conform with ANSI standard FORTRAN language, certain aspects of usage in OZIPM-4 are not compatible on all computer systems. The variable UROUND in BLOCK DATA should be set to the round-off error associated with each computer system. Currently, UROUND is set to the round-off error of 2.4×10^{-7} associated with a PRIME 750 computer system. To reset UROUND, the line in the BLOCK DATA routine should be changed as follows:

```
DATA   UROUND/user's round-off error/
```

UROUND is calculated form the number of significant digits (N) used for the mantissa of a floating point constant:

$$\text{UROUND} = 2^{-N}.$$

For the PRIME 750 computer, each word contains 32 BITs, of which 22 are used for the mantissa. Thus, 2^{-22} is equal to approximately 2.4×10^{-7}. This is the value currently set in OZIPM-4.

Another variable in OZIPM-4 that is machine-dependent is EXPMAX, which is found in subroutines CURV1 and KURV1. This variable represents the maximum possible value for the exponent of e. For the PRIME computer, the range of the real constants is from 10^{-38} to 10^{38}. Hence, the maximum value for the exponent of e is

$$e^{\text{EXPMAX}} = 10^{38},$$

i.e., EXPMAX is 87.4 for the PRIME computer, the value currently set in OZIPM-3. To reset EXPMAX, the user must change the line located in BLOCK DATA accordingly:

```
DATA EXPMAX/user's maximum exponent/
```

The OZIPM-4 prints the input file on the output file so that users can easily see any problems with the input file. To do this, the input file (FORTRAN unit 5) must be rewound. Some computer systems do not allow a rewind option on the input file. If this is the case, lines A125-A136 in the MAIN routine should be taken out. Some computer systems do not allow arguments to be in a mixed mode (i.e., a REAL variable declared as INTEGER in separate subroutines). If this is the case, line AG13 in subroutine NSSFAC must be modified to REAL instead of INTEGER. The OZIPM-4 source code can be computed with either ANSI FORTRAN-66 or ANSI FORTRAN-77 provided the following steps are taken:

For ANSI-FORTRAN-66 compilations:

The SAVE statement found in every subprogram must be either completely deleted from the source file or commented out by placing a "C" in column 1.

For ANSI-FORTRAN-77 compilations:

Some sections of the OZIPM-4 program require a 1-trip DO loop option. Current ANSI FORTRAN-77 performs a zero-trip DO loop if the second argument is less than the first argument. Most compilers allow a 1-trip DO loop by setting a compiler switch. This should be done in ANSI FORTRAN-77 compilations if the switch is available.

Use of CALCOMP Routines

The CALCOMP routines required by OZIPM-4 are

```
Subroutine PLOT (XX,YY,IX)
           PLOTS (XX,UU,IX)
           SYMBOL (XX,YY,HT,ITX,ANG,NCH)
           NUMBER (XX,YY,HT,FPN,ANG,NDEC)
           NEWPEN (IPEN)
```

For users without access to these CALCOMP routines, dummy routines may be needed to run OZIPM-4. To generate the dummy routines, the user must have the following cards for each of these CALCOMP routines:

```
SUBROUTINE_________(argument list)
RETURN
END
```

For users with access to standard CALCOMP routines, no modifications to OZIPM-4 are required. The user should check to ensure that the five routines in their system have the same names as those given above.

Control Language--

Since the job control language necessary to run OZIPM-4 is different for each computer system, only the files required by the program are discussed in this section. Table 9 lists the files and the FORTRAN file unit numbers used by OZIPM-4.

TABLE 8. Input Format for OZIPM-4 Options.

Option	Line No.	Column	Contents
MECHANISM	A kinetic mechanism may be input with this option		
	1	1-4	MECH
		5-10	Not read
		11-20	The identification number on the last reaction line to be read in (MAX = 135) If a negative number is entered, then the default mechanism will be printed
		21-30	The number of photolysis reactions found in the mechanism (MAX is 20; DF = 10)
		31-40	Number of organic species in the 0600-0900 ambient mix (MAX = 20; DF = 9)
		41-50	Chemical reaction format (nonzero for CHEMK format; DF = nonunity stoichiometric coefficient format)
		51-60	The temperature (in degrees K) used for the simulations (DF = 303)
		61-80	Not read
	2	1-10 11-20 . . .	The list of reaction numbers identifying the photolysis reactions in the kinetic mechanism (up to seven on a line). Continue on next line (if necessary)
		61-70	
		71-80	Not read
	3	1-4	The list of names (or alphanumeric symbol) for the set of organic species Continue on next line (if necessary)
		61-64	
		65-68	Not read

TABLE 8 (continued)

Option	Line No.	Column	Contents
MECHANISM	4	1-10 . . . 61-70	The list of the number of carbons associated with each of the organic species. Must be in the same order as the organic species name vector on the previous line(s). Continue on next line (if necessary)
		71-80	Not read
	The mechanism is entered next.		
	There are two formats:		
	5+(CHEMK format)	1-3	The identification number of the reaction (right-justified integer); number may be between 1 and 135
		6-9 11-14 16-19	The names of the reactants (up to three allowed); left-justified
		21-24 26-29 31-34 36-39	The names of the products (up to four allowed); left-justified
		41-50	The rate constant at 298 K or the multiplicative factor for photolysis reactions (right-justified if E-format)
		51-60	The activation energy (in degrees K) if there is one (right-justified if E-format)
	5+(nonunity stoichiometric coefficient format)	1-4 7-10 13-16	The names of the reactants (up to 3 allowed); left-justified
		17-19	The identification number for the reaction (right-justified integer); MAX = 135
		20-24	Coefficient for 1st product (DF = 1.)
		25-28	Name of 1st product; left-justified
		29	An '*' in this column means that there will be additional (up to 6 more) products on the next line

TABLE 8 (continued)

Option	Line No.	Column	Contents
MECHANISM		31-35	Coefficient for 2nd product (DF = 1.)
		37-40	Name of 2nd product; left-justified
		43-47	Coefficient for 3rd product (DF = 1.)
		49-52	Name of 3rd product; left-justified
		55-64	The rate constant at 298 K or the photolysis multiplicative factor
		66-72	The activation energy (in degrees K)
	The next card is used when more than 3 products are in the reaction.		
		1-5	Coefficient for 4th product (DF = 1.)
		7-10	Name of 4th product; left-justified
		13-17	Coefficient for 5th product (DF = 1.)
		19-22	Name of 5th product; left-justified
		25-29	Coefficient for 6th product (DF = 1.)
		31-34	Name of 6th product; left-justified
		37-41	Coefficient for 7th product (DF = 1.)
		43-46	Name of 7th product; left-justified
		49-53	Coefficient for 8th product (DF = 1.)
		55-58	Name of 8th product; left-justified
		61-65	Coefficient for 9th product (DF = 1.)
		67-70	Name of 9th product; left-justified

TABLE 8 (continued)

Option	Line No.	Column	Contents
ZENITH*			Revise or input photolysis rates as a function of solar zenith angle. This option is required when an optional mechanism is used. This option can also be used with the default mechanism (1) to vary the photolysis rates in a fashion independent from NO_2 photolysis for those reactions that are presently assumed to photolyze like NO_2 or (2) to modify the default values for the zenith angle dependence of NO_2, $O_3 \rightarrow O\ (^1D)$, FORM, ALD2, H_2O_2, OPEN, and MGLY. Note that photolytic reactions that vary with zenith angle in a fashion similar to NO_2 need not be entered.
	1	1-4	ZENI
		5-10	Not read
		11-20	Number of photolysis reactions with zenith angle dependence.
			The next two lines are repeated for each photolysis reaction. The order of the photolysis rates represents values for the following zenith angles: 0., 10., 20., 30., 40., 50., 60., 70., 78., 86.
	2	1-10	Photolysis reaction number
		11-20 21-30 31-40 41-50 51-60 61-70	Photolytic ratios relative to NO_2 for the first six zenith angles.
	3	1-10 11-20 21-30 31-40	Photolytic ratios relative to NO_2 for the last four zenith angles.

---

* Default values for the photolysis species in the CBM-IV are given in Tables 2-4 (Section 4).

TABLE 8 (continued)

Option	Line No.	Column	Contents
TITLE	Input a new title. If this option is not activated, the default title is "Standard Ozone Isopleth Conditions."		
	1	1-4	TITL
	2	1-72	The title can be placed anywhere in line between columns 1-72

TABLE 8 (continued)

Option	Line No.	Column	Contents
PLACE	Input city-specific information on light intensity. Default values correspond to Los Angeles on 21 June 1986.		
	1	1-4	PLAC
		11-20	Latitude, in decimal degrees north of the equator (DF = 34.058)
		21-30	Longitude, in decimal degrees west of Greenwich meridian (DF = 118.250)
		31-40	The time zone, in hours from Greenwich mean time (DF = 7.0)
		41-50	The year (DF = 1986)
		51-60	The month of year (DF = 6)
		61-70	The numerical day of month (DF = 21)
	2 (optional)	1-24	The name of the place can be entered anywhere in columns 1-24. Include this line only if a new value is entered for the latitude or longitude on the previous line

TABLE 8 (continued)

Option	Line No.	Column	Contents
MIXING	Option for use when data on hourly mixing heights are available. Mixing heights are read for the initial height and the height at the end of each hour. If dilution occurs for n hours, there should be n+1 mixing heights.		
	1	1-4	MIXI
		11-20	Number of hours (n) of dilution (MAX = 24)
		21-30	Mixing height at time t = 0
		31-40	Mixing height at time t = 1 hr
		41-50	Mixing height at time t = 2 hr
		51-60	Mixing height at time t = 3 hr
		61-70	Mixing height at time t = 4 hr
		71-80	Not read
			If more than 4 hours of dilution, continue on next line
	2+ (optional)	1-10 . . . 61-70	Continuation of mixing heights
		71-80	Not read

TABLE 8 (continued)

Option	Line No.	Column	Contents
DILUTION	Read site-specific information on initial and final mixing heights. Dilution is calculated using the characteristic curve.		
	1	1-4	DILU
		11-20	Initial mixing height, Z1, in any units (DF = 510 m)
		21-30	Final mixing height, Z2, in same units as initial mixing height (DF = 630 m)
		31-40	Starting time of mixing height change (2400 hour) (DF = 800)
		41-50	Ending time of mixing height change (2400 hour) (DF = 1500)
		51-60	Dilution rate in percent per hour before and after the mixing height change (DF = 0)
		61-80	Not read

TABLE 8 (continued)

Option	Line No.	Column	Contents
TEMPERATURE	A varying temperature profile may be used during the simulation with this option. Temperature values should be in units of degrees K. Values are read for the initial time and at the end of each hour. If there are n hours, there should be n+1 temperature values.		
	1	1-4	TEMP (DF = 303 K)*
		11-20	Number of hours (n) of varying temperature (MAX = 24)
		21-30	Temperature at time t = 0
		31-40	Temperature at time t = 1 hr
		41-50	Temperature at time t = 2 hr
		51-60	Temperature at time t = 3 hr
		61-70	Temperature at time t = 4 hr
		71-80	Not read
			If more than 4 hours of values, continue on next line
	2+ (optional)	1-10 . . . 61-70	Continuation of temperature values
		71-80	Not read

---

* If the user desires a new constant temperature value, this can be implemented using the MECH option.

TABLE 8 (continued)

Option	Line No.	Column	Contents
TRANSPORT	Option for site-specific information on O_3, NO_2, and NMOC transported in the surface layer and in the air aloft that is entrained as the inversion rises. (If TRAN option is not used, concentration of transported species is 0.)		
	1	1-4	TRAN
		11-20	Transported ozone concentration in the surface layer
		21-30	Ozone entrained from aloft
		31-40	If nonzero and positive:[*] Transported NMOC in the surface layer. If nonzero and negative: Number of NMOC species in the 0600-0900 mix
		41-50	If nonzero and positive:[*] Total NMOC entrained from aloft. If nonzero and negative: Number of NMOC species in the 0600-0900 mix
		51-60	Transported NO_2 in the surface layer
		61-70	NO_2 entrained from aloft
		71-80	Not read
	2 (optional)	1-10	If a nonzero negative value is entered in columns 31-40 of the TRAN line, the total NMOC transported in the surface layer is entered here (ppmC).
		11-20 . . .	The fraction of the total NMOC for each of the organic species transported in the surface layer (should be in the same order as listed in the MECH option).[‡]
		61-70	Continue on next line (if necessary)
		71-80	Not read

---

[*] Can only be used with the CBM-IV. The default carbon fractions for NMOC transport in the surface layer and for NMOC aloft are given in Table 5, Section 4.

[‡] The default order of the NMOC species in CBM-IV is: ETH, OLE, ALD2, FORM, TOL, XYL, PAR, ISOP, and NR.

TABLE 8 (continued)

Option	Line No.	Column	Contents
TRANSPORT	3 (optional)	1-10	If a nonzero negative value is entered in columns 41-50 of the TRAN line, the total NMOC entrained from aloft is entered here (ppmC)
		11-20 . . . 61-70	The fraction of the total NMOC entrained for each of the organic species entrained from aloft (should be in the same order as listed in the MECH option). Continue on next line (if necessary)
		71-80	Not read

TABLE 8 (continued)

Option	Line No.	Column	Contents
INITIAL	Molecular concentrations of species other than O_3, NO_2, and NMOC that are transported in the surface layer can be entered with this option.		
	1	1-4	INIT
		11-20	Number of transported species with nonzero concentrations (DF = 0; MAX = 60)
		21-80	Not read
	2	1-4 11-14 21-24 31-34 41-44 51-54 61-64	The list of names of the transported species with nonzero concentrations (continue on next line if necessary)
		65-80	Not read
	3	1-10 11-20 . . . 61-70	The molecular concentrations for the species listed on the previous line(s) (ppm)
		71-80	Not read

TABLE 8 (continued)

Option	Line No.	Column	Contents
ALOFT	Molecular concentrations of species other than NMOC, NO_x, and O_3 in the aloft layer can be entered with this option.		
	1	1-4	ALOF
		11-20	Number of species with nonzero aloft concentrations (DF = 0; MAX = 10)
		21-80	Not read
	2	1-4 11-14 21-24 31-34 41-44 51-54 61-64	The list of names of the species with nonzero aloft concentrations (continue on next line if necessary)
		65-80	Not read
	3	1-10 11-20 . . . 61-70	The aloft molecular concentrations for the species listed on the previous line (ppm)
		71-80	Not read

TABLE 8 (continued)

Option	Line No.	Column	Contents
BACKGROUND	Background concentrations* of NMOC, NO_2 and O_3 can be set with this option. (If background option is not used, the minimum background levels are zero.)		
	1	1-4	BACK
		11-20	Background concentration of O_3 (ppm)
		21-30	If nonzero and positive: The background concentration of NMOC (ppmC) for the CBM-IV chemistry If nonzero and negative: The number of organic species in the optional mechanism
		31-40	Background concentration of NO_2 (ppm)
	2 (optional)	1-10	Background concentration of NMOC (ppmC)
		11-20 21-30 31-40 41-50 51-60 61-70	If a nonzero negative number is entered in columns 21-30 of line 1, the fraction of the total background NMOC for each of the organic species (should be in the same order as listed in the MECH option). Continue on next line (if necessary)

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* Minimum levels for transport concentrations in the surface and aloft layers.

TABLE 8 (continued)

Option	Line No.	Column	Contents
EMISSIONS	Input city-specific information on post-0800 emissions.		
	1	1-4	EMIS
		11-20	The number of hours for which emission fractions are to be input, from 1.0 to 24.0 (DF = 0). This number should be coded as positive if the same fractions for NMOC and NO_x are to be used. It should be coded as negative if different fractions are to be used
		21-30	NMOC or NMOC and NO_x emission fraction for hour 1 (DF = 0). If all NMOC fractions are to be set to zero, enter any negative number and skip to record 3
		31-40	NMOC or NMOC and NO_x emission fraction for hour 2 (DF=0)
		. . .	
		61-70	NMOC or NMOC and NO_x emission fraction hour 5 (DF = 0)
	The following line is included and repeated if more than five hours of emissions are specified.		
	2 (optional)	1-10	NMOC or NMOC and NO_x emission fraction for hour 6
		11-20	NMOC or NMOC and NO_x emission fraction for hour 7
		. . .	
		61-70	NMOC or NMOC and NO_x emission fraction for hour 12
	The next line is included when separate NMOC and NO_x fractions are specified. This line is repeated when the number of hours of emissions is greater than 7.		
	3 (optional)	1-10	NO_x emission fraction for hour 1. If all NO_x fractions are set to zero, then any negative number should be entered, and no further entries are required

TABLE 8 (continued)

Option	Line No.	Column	Contents
EMISSIONS		11-20	NO_x emission fraction for hour 2
		.	
		.	
		.	
		61-70	NO_x emission fraction for hour 7
	4 (optional)	1-10	NO_x emission fraction for hour 8
		11-20	NO_x emission fraction for hour 9
		.	
		.	
		.	
		61-70	NO_x emission fraction for hour 14

TABLE 8 (continued)

Option	Line No.	Column	Contents
MASSEMISS	Used to supply mass emission densities through which post-0800 emission fractions are computed		
	1	1-4	MASS
		11-20	Number of hours of emissions (max = 24.) (expressed as a negative number)
		21-30	Measured 0600-0900 NMOC concentration used to compute NMOC emission fractions, ppmC
		31-40	Measured 0600-0900 NO_x concentration used to compute NO_x emission fractions, ppm
		41-50	Mixing height at start of simulation, in meters
	The next line is repeated if more than 7 hours of emissions are specified. The number of entries must equal the number of hours specified on line 1.		
	2	1-10	VOC emission density for hour 1, kg/km^2
		11-20	VOC emission density for hour 2, kg/km^2
		⋮	
		61-70	VOC emission density for hour 7, kg/km^2
	The next line is repeated if more than 7 hours of emissions are specified. The number of entries must equal the number of hours specified on line 1.		
	3	1-10	NO_x emission density for hour 1, kg/km^2
		11-20	NO_x emission density for hour 2, kg/km^2
		⋮	
		61-70	NO_x emission density for hour 7, kg/km^2

TABLE 8 (continued)

Option	Line No.	Column	Contents
MOLEMISS	Incorporate site-specific information on emissions of up to 5 species including VOC and NO_x. Note VOC and NO_x emissions are required with this option and should be the first and second species listed.		
	1	1-4	MOLE
		11-20	Number of hours during which emissions occur; from 1 to 24 (DF = 0); the negative value should be entered
		21-30	Number of species that have emission rates (MAX = 5)
		31-40	If nonzero: The initial mixing height used for conversion of moles to ppm units (units should be consistent with the mixing height units entered in the DILU or MIXI options)
		41-50	If nonzero, the horizontal area used to convert emissions in moles to ppm units (units for the area should be consistent with the mixing height units)
		51-60	The measured 0600-0900 NMOC concentration used to compute NMOC emission fractions, ppmC
		61-70	The measured 0600-0900 NO_x concentration used to compute NO_x emission fractions, ppm
			If there are emissions of species other than VOC or NO_x, then line 2 contains the 0600-0900 concentration of each species.
	2	1-10	Measured 0600-0900 concentration of the third species, ppm
		11-20	
		⋮	
		21-30	

TABLE 8 (continued)

Option	Line No.	Column	Contents
	The next set of lines is repeated for each species with emissions.		
	3+	1-4	Species name (use VOC for VOC emissions, NOX for nitrogen oxides emissions)
		11-20 21-30 . . .	Emission rates in units of ppm/hr or moles/hr (ppmC or moles C for VOC emissions)
		61-70	If more than 5 hours of continuous emissions are to be entered, continue on next line.

TABLE 8 (continued)

Option	Line No.	Column	Contents
DEPOSITION	Incorporate information on species deposition.		
	1	1-4	DEPO
		11-20	Number of hours during which deposition occurs; from 1 to 24; DF = 0
		21-30	Number of species that have deposition rates; MAX = 5
	The next set of lines is repeated for each species with deposition rates.		
	2	1-4	Species name (use NMOC for NMOC deposition) (NO and NO_2 deposition are treated separately)
		11-20	Deposition velocity for hour 1, cm/s
		21-30	Deposition velocity for hour 2, cm/s
		.	.
		.	.
		.	.
		61-70	Deposition velocity for hour 6, cm/s
	If more than 6 hours of deposition are to be entered, continue on next line.		

TABLE 8 (continued)

Option	Line No.	Column	Contents
REACTIVITY*			Contains site-specific information on organic reactivity and NO_2/NO_x ratio for the initial 6-9 AM mix and the VOC and NO_x emissions.
	1	1-4	REAC
		5-10	Not read
		11-20	The number of organic species in the 0600-0900 mix
		21-30	The NO_2/NO_x fraction
	2	1-10 . . . 61-70	The reactivity for each of the organic species (up to 7 on a line) represented as the fractions of total NMOC. Continue on next line (if necessary)
		71-80	Not read

---

* If the REACTIVITY option is not used, the default fractions are those shown in Table 6, Section 4.

TABLE 8 (continued)

Option	Line No.	Column	Contents
TIME	Reset starting and ending times for simulations with this line.		
	1	1-4	TIME
		5-10	Not read
		11-20	Starting time for simulations based on 24-hour clock (DF = 800)
		21-30	Ending time for simulations (DF = 1800). Note: Maximum difference is 24 hours
		31-80	Not read

TABLE 8 (continued)

Option	Line No.	Column	Contents
RATE	Rate constant changes are implemented with this option.		
	1	1-4	RATE
		5-10	Not read
		11-20	Number of rate constants to be changed
		21-30	Special option for testing emissions, photolysis, dilution, etc. A nonzero number sets all reaction rate constants to zero except photolysis reactions
	2 (optional)	1-10 . . . 61-70	Identification numbers for the reactions with rate constants to be changed (each reaction number in each 10-column field)
		71-80	Not read
	3 (optional)	1-10 . . . 61-70	List of the new rate constants (must be in the same order as entered on line 2). Each rate constant in each 10-column field (right-justified if E format)
		71-80	Not read

TABLE 8 (continued)

Option	Line No.	Column	Contents
SPECIES	This option allows the user to plot isopleths for any species found in the kinetic mechanism or to plot concentration-time profiles for species besides O_3 if the CALCULATE option is used.		
	1	1-4	SPEC
		11-20	Number of species to be plotted (MAX = 5; DF = 1)
		21-80	Not read
		1-4 11-14 21-24 31-34 41-44	The alphanumeric symbol of the species of interest; left-justified (DF = 03 [ozone])
		45-80	Not read

TABLE 8 (continued)

Option	Line No.	Column	Contents
ACCURACY	Increase or reduce the mathematical accuracy of the isopleth diagram by increasing or decreasing the accuracy of the numerical integration scheme, more or less accurate interpolation, etc.		
	1	1-4	ACCU
		11-30	Not read
		31-40	Error tolerance in the numerical integration routine, from 0.1 to 0.00001; (DF = 0.003)
		41-50	Tension factor for hyperbolic spline functions used in first stage of interpolation from 0.001 to 50.; (DF = 1)
		51-60	Tension factor for hyperbolic spline functions used in plotting isopleth lines (high tensions lead to straight lines drawn between the points obtained from the first stage), from 0.001 to 50.; (DF = 1)
		61-70	If any nonzero value is entered in this field, simulations will terminate after any ozone maximum; no entry produces results over the total simulation period

TABLE 8 (continued)

Option	Line No.	Column	Contents
ALREADY*	Include results from a previous run.		
	1	1-4	ALRE
		11-20	Number of previous simulations to be input If the number is positive, then read the following lines. If the number is negative, then read previous simulation results from an external file
	2	1-10	NMOC concentration
		11-20	NO_x concentration
		21-30	Maximum one-hour average ozone concentration, ppm
		31-40 41-50 51-60 61-70	Maximum one-hour average species concentrations (ppm) of any other species for which isopleths are to be plotted. These values are optional depending on the number of species declared on the SPECIES line. (Must be in the same order as listed on the SPECIES line.)

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* Can be used only with the ISOPLETH option.

TABLE 8 (continued)

Option	Line No.	Column	Contents
PLOT	Activates the drawing of the isopleth diagram on an off-line plotter.		
	1	1-4	PLOT
		11-20	Scaling factor for the location of labels for each ozone isopleth. The value should be between 0.1 and 0.8.; (DF = 0.6)
		21-30	If nonzero, a grid is overlaid onto the diagram. If the value is positive and nonzero, a grid is overlaid on the diagram using a different color pen (if available) If the value is negative, a grid with line of different patterns (e.g., dot-dash) is overlaid on the plot. The absolute value of this number corresponds to different patterns and textures
		31-40	Length (in inches) of the abscissa (NMOC scale) of the isopleth diagram; (DF = 8.5)
		41-50	Length (in inches) of the ordinate (NO_x scale) of the isopleth diagram; (DF = 5.95)
		51-60	Size (in inches) of the numbers to be printed on the axes and of the characters in the title; (DF = 0.10)
		61-70	The size (in inches) of the labels on the ozone isopleths and the division marks on the axis; (DF = 0.07)

TABLE 8 (continued)

Option	Line No.	Column	Contents
CREDIT			Allow for post-0800 CO emissions in EKMA calculations. If the CRED option is not used, defaults are no post-0800 CO emissions, 1.2 ppm CO for the 0600 to 0900 concentration, and 0.5 ppm CO aloft with no change in future year levels.
	1	1-4	CRED
		11-20	Enter a negative number to defeat option in multiple runs (DF=0)
		21-30	Number of emission hours. Must be equal to number of hours set in EMIS, MASS, or MOLE options. If the value is positive then the CO emissions are entered as fractions of the 0600-0900 CO concentration. If the value is negative, the CO emissions are in mass units of kg/km^2.
		31-40	Initial mixing height. Used only when mass units are input
	2	1-10	Species name. CO is the only name allowed.
		11-20	0600-0900 present-day CO concentration (DF=0)
		21-30	Not read
		31-40	Present-day CO transported aloft (DF = 0.0)
		41-50*	Percent change in CO emissions and 0600-0900 CO concentrations for the future year
		51-60	Not read
		61-70*	Future-year CO transported aloft
	3+	1-10 11-20... . . . 61-70	Present-day hourly emissions of CO (continue on next line if necessary)

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* Not used with CALC and ISOP options.

TABLE 8 (continued)

Option	Line No.	Column	Contents
CALCULATE	Perform a single simulation with the initial NMOC and NO_x concentrations specified on this line.		
	1	1-4	CALC
		11-20	0600-0900 NMOC concentration
		21-30	0600-0900 NO_x concentration
		31-40	Information option; entry of any nonzero value will result in printing of the computed concentrations of all species, the rate of change of all species, reaction rates, etc. Photolysis constants are also printed
		41-50	Time (in minutes) from the beginning of the simulation at which computed concentrations of all species in the kinetic mechanism are to be printed; (DF = 60)
		51-60	Time step (in minutes) for subsequent printing of concentrations; (DF = 60)

TABLE 8 (continued)

Option	Line No.	Column	Contents
EKMA	Used to perform a VOC emission requirement calculation		
	1	1-4	EKMA
		11-20	Base-case ozone concentration, ppm
		21-30	NMOC/NO_x ratio (If the value is negative, the base-year NMOC and NO_x levels have been determined in a previous simulation and are entered on line 3. Future-year calculations are performed based on the base-year NMOC and NO_x levels.)
		31-40	Percent change in NO_x emissions; positive number for increase, negative number for decrease (DF = 0)
		41-50	Future transport indicator; if nonzero, input record 2 is required (DF = 0)
		51-60	Option to generate report of change in ozone as a function of change in VOC emissions; if 1., generate tabular report; if 2., generate tabular report and write results to file. (DF = 0., i.e., no report or file generated)
		61-70	Flag to do a calculation at a specified NMOC level. The NMOC level is expressed as a percent change from the base-year level. The value is placed on line 3, columns 41-50.
	The next line is included only if a nonzero entry is specified for the future transport indicator (41-50).		
	2 (optional)	1-10	Concentration of ozone transported in surface layer for post-control conditions, ppm; (DF = 0). A negative value activates the use of the future ozone transport estimate curves shown in Figure 4. (A value less than -100 activates the use of the dotted line shown in Figure 4.)
		11-20	Concentration of ozone transported aloft for post-control conditions, ppm; (DF = 0). A negative value activates the use of the future ozone transport estimate curves shown in Figure 4. (A value less than -100 activates the use of the dotted line shown in Figure 4.)

TABLE 8 (continued)

Option	Line No.	Column	Contents
EKMA	2	21-30	Concentration of NMOC transported in the surface layer for post-control conditions, ppmC; (DF = 0). The absolute value of the negative number entered represents the median contribution factor as described in Appendix B of EPA (1981).
		31-40	Concentration of NMOC transported aloft for post-control conditions, ppmC; (DF = 0). The absolute value of the negative number entered represents a 40% reduction in present-day NMOC aloft
		41-50	Concentration of NO_x transported in surface layer for post-control conditions, ppm; (DF = 0).
		51-60	Concentration of NO_x transported aloft for post-control conditions, ppm; (DF = 0).

The following line must be included even if the default values of 0 are used for all parameters.

Option	Line No.	Column	Contents
	3	1-10*	Measured 0600-0900 NMOC (Value used in emission density calculations) (DF = 0.)
		11-20*	Measured 0600-0900 NO_x (Value used in emission density calculations) (DF = 0.)
		21-30	Calculated NMOC that yields base-case O_3. Declared if a negative NMOC/NO_x ratio is entered on line 1. (DF = 0.)
		31-40	Calculated NO_x that yields base-case O_3. Declared if a negative NMOC/NO_x ratio is entered on line 1. (DF = 0.)
		41-50	Change in NMOC level (percent) for specific calculation after the base-year ozone is estimated (used only if column 61-70 of line 1 is nonzero).

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* Must be specified so that OZIPM-4 can determine the location of the base-year ozone should two or more base-year ozone values occur along a NMOC/NO_x line. Values must agree with those specified in MASS or MOLE option.

TABLE 8 (continued)

Option	Line No.	Column	Contents
ISOPLETH			Construct isopleth diagram(s) for O_3 and other species according to the input parameters. Default isopleths for O_3 are 0.08, 0.12, 0.16, 0.20, 0.24, 0.28, 0.30, 0.32, 0.34, 0.36 and 0.40 ppm.
	1	1-4	ISOP
		11-20	Maximum NMOC concentration on abscissa of isopleth diagram; (DF = 2.0 ppmC)
		21-30	Maximum NO_x concentration on ordinate of isopleth diagram; (DF = 0.28 ppm)
		31-40	Number of ozone isopleths to be drawn, from 1. to 20.; (DF = 11)
		41-50	Any nonzero value will activate the printing of solar noon and the time of the center of the maximum one-hour average ozone concentration for each simulation
		51-60	Not read
		61-70	Number of species to plot. This number corresponds to the number of species entered on the SPECIES option
	2 (optional)	1-10	Ozone concentration of 1st isopleth, ppm
		11-20	Ozone concentration of 2nd isopleth, ppm
		21-30	Ozone concentration of 3rd isopleth, ppm
		31-40	Ozone concentration of 4th isopleth, ppm
		41-50	Ozone concentration of 5th isopleth, ppm
		51-60	Ozone concentration of 6th isopleth, ppm
		61-70	Ozone concentration of 7th isopleth, ppm

TABLE 8 (continued)

Option	Line No.	Column	Contents
ISOPLETH	3 (optional)	1-10 . . .	Ozone concentration of 8th isopleth, ppm
		61-70	Ozone concentration of 14th isopleth, ppm
	4 (optional)	1-10 . . .	Ozone concentration of 15th isopleth, ppm
		51-60	Ozone concentration of 20th isopleth, ppm
	5+		Lines 2-4 are repeated for each additional species to be plotted (must be in some order as listed on the SPECIES option).

TABLE 8 (concluded)

Option	Line No.	Column	Contents
bbbb	A blank line must follow all input options to terminate the program.		
	1	1-4	Blanks

TABLE 9. Files Used by OZIPM-4.

File	FORTRAN Unit*	Read(R)/ Write(W)	Comment
Input file	5	R	The card input deck
Output file	6	W	The output of the OZIPM-4 results
ALREADY file	9	W	The results of each simulation on a diagram point are written to this file for later use
ALREADY file	8	R	File of results from a previous run used to continue an isopleth simulation or redo the isopleth
PLOT file (optional)	--	W	The file to which CALCOMP or offline plots are written. The file unit is dependent on the computer system
EKMA file (optional)	11	W	The file to which EKMA calculations are written when the option flag in columns 51-60 on the <u>EKMA</u> line is set to 2.

---

* Each of the unit numbers can be changed in the OZIPM-4 program by modifying the following statement in the BLOCK DATA routine:

```
DATA IN/5/, IOUT/6/, IALN/9/, IALL/8/, IOZC/11/.
```

6 EXAMPLES OF OZIPM RUNS

Five examples of how to use OZIPM-4 with the CBM-IV and optional mechanisms are presented in this section. Exhibits 1 through 10* show the input and output files for each example. Each example is discussed in detail.

Example 1

Example 1 illustrates the use of the default CBM-IV mechanism with a set of city-specific information described by PLACE, DILUTION, EMISSIONS, and TRANSPORT options. Exhibit 1 shows the input file for this example. (The first three lines in this exhibit are used to orient the user by providing column numbers.) A single simulation is performed using the CALCULATE option at a NMOC value of 1.0 ppmC and a NO_x value of 0.10 ppm. Also note that there is a nonzero value in columns 31-40 of the CALCULATE option, which will result in a detailed printout of the simulation. The SPECIES option is used in this simulation so that plots of maximum hourly-averaged concentrations of NO_2 and PAR can be obtained along with the plot of the maximum hourly-averaged O_3 concentration.

The output from this simulation is shown in Exhibit 2. The first page of the output describes the version of OZIPM-4 being used. The second page is a printout of the input stream. This feature is provided so that users may readily review the input information associated with the simulation output. The default mechanism and the photolysis rates are printed next because a value of -1 was placed on the MECHANISM option. The next two pages are header pages that describe the inputs used in this simulation. The following pages contain the detailed simulation results for each hour of the simulation. At the end of the simulation is a summary of the maximum O_3, NO_2, and PAR concentrations found in the simulation. Three plots (one each for O_3, NO_2, and PAR) in the output show the temporal behavior for each species of interest.

---

* For the convenience of the user, Exhibits 1 through 10 are presented at the end of this section.

Example 2

Example 2 illustrates the use of the CALCULATE option for a chemical mechanism. In this example, the default CBM-IV mechanism is input with one additional reaction to treat methanol (Reaction 83; see Exhibit 3). Exhibit 3 shows the input deck for this simulation. The inputs for this example are comparable to those for example 1, with the additional options TEMPERATURE, MOLE, DEPOSITION, INITIAL, ALOFT, AND REACTIVITY invoked. The chemical mechanism is implemented through the use of the MECHANISM option. Following the MECHANISM line is (1) the list of photolysis reactions, (2) the list of the organic species, and (3) the carbon number of each organic species. The chemical reactions are input next.

The ZENITH option follows the MECHANISM option. The zenith angle dependence for each photolysis reaction is entered beginning at 0(zero) degrees. Only seven photolysis reactions are input even though there are a total of eleven photolysis reactions. Reactions 8, 14, and 23 have zenith-angle dependences similar to those of NO_2 photolysis. Since the photolysis rate constants for these reactions are constant ratios to NO_2 photolysis, their zenith-angle dependence does not need to be input with the ZENITH option.

Following the ZENITH option are the city-specific options described in Example 1. This example illustrates the use of the MOLE option when post-0800 emissions are in units of moles $m^{-1}hr^{-1}$. In this example, surface depositions of NO, NO_2, and O_3 are treated explicitly. The DEPOSITION option shown in EXHIBIT 3 is used for illustrative purposes only. In realistic simulations, the deposition rate will vary with different surface types. The INITIAL option is used to input H_2O and CO concentrations other than the default values stored within the program. The ALOFT option is used to input PAN and CO transported aloft. The value entered for CO overrides the default value of 0.5 ppm stored within the program. The output is shown in Exhibit 4. Note that for this example CO concentrations can be entered using the CREDIT option, but the user would have to enter post-0800 emissions of CO. This example assumes zero post-0800 CO emissions. The output formats are similar to those given in Example 1.

Example 3

Example 3 illustrates the use of the EKMA option to predict the actual reduction in VOC emissions needed to reach the NAAQS of 0.12 ppm. Exhibit 5 shows the input file for this example. This example also illustrates the use of the MASS and CREDIT options. The MASS option allows the user to input mass emission densities in units of kg/km^2. The first line in the MASS option contains the negative number of hours of emissions, followed by the measured 0600-0900 NMOC and NO_x concentrations, and the initial mixing height. Note that the mixing height must be in meters. The next lines contain the mass emissions of VOC and NO_x. The CO CREDIT option is used to specify post-0800 CO emissions. The CREDIT line (line 15 in Exhibit 5) contains the negative number of hours of emissions, followed by the initial mixing height. A negative value is used to indicate that mass emission densities are used in the following lines. The next line contains the name of the species (CO is the only name allowed) followed by the measured 0600-0900 concentration, the present-year concentrations of CO transported aloft, the percent change in CO emissions in the future year, and the future year CO concentrations transported aloft. The next lines contain the hourly CO emissions followed by the EKMA option. The base-case ozone is 0.17 ppm, the NMOC/NO_x ratio is 10, and the NO_x emissions are reduced by 10.0 percent for the future year. The nonzero flag in columns 41-50 of the EKMA option is used to specify non-zero transport concentrations in the future year. The range option on the EKMA line is invoked on columns 51-60 to give ozone levels at varying VOC reductions. The nonzero value in columns 61-70 tells OZIPM-4 to do a calculation for the future year at a specific NMOC level. The next line after the EKMA line determines the change in transport for the future year. The first two fields, columns 1-10 and 11-20, specify the future-year ozone transported in the surface layer and aloft. A negative value is entered to tell OZIPM-4 to use the standard ozone curves described in EPA (1981) and shown in Figure 4.

The future year NMOC transported in the surface layer and aloft is input in columns 21-40 and 31-40, followed by the future year NO_x transported in the surface layer and aloft (columns 41-50 and 51-60). The third line contains the measured 0600-0900 NMOC and NO_x concentrations. The 0600-0900 NMOC and NO_x concentrations are used within the EKMA option to determine the location of the base-year ozone closest to the measured concentrations should a maximum or minimum occur along the NMOC/NO_x line. The last field (columns 41-50) contains the specific NMOC level at which the future calculation will be performed. The output for this example is shown in Exhibit 6. The output formats are similar to the output from the previous examples except that the simulations required to make the VOC requirement estimate are printed. Note that OZIPM-4 will search for the NMOC and NO_x level along the NMOC/NO_x ratio until it finds the base-case ozone of 0.17 ppm. Then it performs the future year estimate to obtain the VOC control requirement.

Note that in this example NO_x emissions were reduced by 10 percent for the future year. Suppose that we are now interested in determining how much control estimates would change if we were to assume that NO_x

emissions were reduced by 20 percent in the future year. We can save computer time by using EKMA line 3 to specify the NMOC and NO_x concentrations that yielded the base-case ozone value of 0.17 ppm. These values have already been determined and are shown in Exhibit 6. Thus, to run a new simulation, which involves a change only in future-year conditions, we would input the values of 0.46065 and 0.04607 determined for the base-year NMOC and NO_x concentrations in Columns 21-30 and 31-40, respectively, on EKMA line 3.

Example 4

Example 4 is similar to Example 3 except that the NMOC transported in the surface layer must be reduced due to upwind contributions. The procedure outlined in this example is that described in Appendix B of the 1981 EPA guidelines. Exhibit 7 shows the input file for this example. The card following the EKMA card contains the upwind NMOC median contribution factor of 0.32. The contribution factor is entered as a negative number to distinguish it from an absolute concentration. This example illustrates the effects of "overwhelming" transport conditions for which a 100 percent VOC control requirement is not enough to reach the 0.12 ppm standard. In this example the program will stop execution should a 100 percent VOC control requirement be calculated (i.e., the 0600-0900 NMOC location is zero). In cases where transport conditions dominate, the user should generate an isopleth diagram to further examine the model input assumptions. The output for this example is shown in Exhibit 8.

Example 5

Example 5 demonstrates the use of the ISOP option in OZIPM-4. Exhibit 9 shows the input file for this example. The output for this example is shown in Exhibit 10. The output contains the results of the simulations performed for the ISOPLETH option. The ozone isopleth diagram is shown at the end of the output file. Note that the SPECIES option asked for two species (O_3 and NO_2). Thus, the simulations under the ISOPLETH option provide the maximum one-hour values for both species. Isopleth diagrams are generated for both species (Exhibit 10) based on the isolines defined by the user (lines 23 to 26 in Exhibit 9). Note that the user must declare the number of species to be plotted in columns 61-70 on the ISOPLETH line (line 22 in Exhibit 9).

EXHIBIT 1

```
(    1)          1         2         3         4         5         6         7
(    2) 123456789012345678901234567890123456789012345678901234567890123456789012
(    3)
(    4) MECH      -1.
(    5) TITL
(    6) EXAMPLE 1 - SINGLE CALCULATION
(    7) TRANS     .000      .080      0.        .050      0.        0.009
(    8) PLAC      38.629    90.206    5.0       1986.     6.0       21.
(    9) TEST CITY
(   10) DILU      250.      1700.
(   11) EMIS      -11.      .106      .086      .084      .058      .036
(   12) .025      .024      .020      .019      .024      .013
(   13) .343      .262      .239      .174      .117      .080      .081
(   14) .068      .060      .075      .038
(   15) SPEC      3.
(   16) O3        NO2       PAR
(   17) CALC      1.        .1        1.
(   18)     BLANK
(   19)
(   20)          1         2         3         4         5         6         7
(   21) 123456789012345678901234567890123456789012345678901234567890123456789012
```

OZONE ISOPLETH PLOTTING PACKAGE
WITH OPTIONAL MECHANISMS

OZIPM

VERSION 4.00

DECEMBER, 1987

EXHIBIT 2

```
THE INPUTS FOR THIS RUN ARE

         MECH       -1.
         TITL
         EXAMPLE 1 - SINGLE CALCULATION
         TRANS      .000      .080      0.        .050      0.        0.009
         PLAC       38.629    90.206    5.0       1986.     6.0       21.
         TEST CITY
         DILU       250.      1700.
         EMIS       -11.      .106      .086      .084      .058      .036
         .025       .024      .020      .019      .024      .013
         .343       .262      .239      .174      .117      .080      .081
         .068       .060      .075      .038
         SPEC       3.
         03         NO2       PAR
         CALC       1.        .1        1.
```

```
THE REACTIONS                                                                          RATE CONSTANT  ACT. ENERGY(K)
  1       NO2                        =        NO     +      O                           1.000E+00      0.000E+00
  2       O                          =        O3                                        4.323E+06     -1.175E+03
  3       O3    +     NO             =        NO2                                       2.664E+01      1.370E+03
  4       O     +     NO2            =        NO                                        1.375E+04      0.000E+00
  5       O     +     NO2            =        NO3                                       2.309E+03     -6.870E+02
  6       O     +     NO             =        NO2                                       2.438E+03     -6.020E+02
  7       NO2   +     O3             =        NO3                                       4.731E-02      2.450E+03
  8       O3                         =        O                                         5.300E-02      0.000E+00
  9       O3                         =        O1D                                       1.000E+00      0.000E+00
 10       O1D                        =        O                                         4.246E+05     -3.900E+02
 11       O1D   +     H2O            =      2 OH                                        3.260E+00      0.000E+00
 12       O3    +     OH             =        HO2                                       1.000E+02      9.400E+02
 13       O3    +     HO2            =        OH                                        3.000E+00      5.800E+02
 14       NO3                        =   0.89 NO2    + 0.89 O      + 0.11 NO            3.390E+01      0.000E+00
 15       NO3   +     NO             =      2 NO2                                       4.416E+04     -2.500E+02
 16       NO3   +     NO2            =        NO     +      NO2                         5.901E-01      1.230E+03
 17       NO3   +     NO2            =        N2O5                                      1.853E+03     -2.560E+02
 18       N2O5  +     H2O            =      2 HNO3                                      1.900E-06      0.000E+00
 19       N2O5                       =        NO3    +      NO2                         2.776E+00      1.090E+04
 20       NO    +     NO             =      2 NO2                                       1.539E-04     -5.300E+02
 21       NO    +     NO2   +   H2O  =      2 HNO2                                      1.600E-11      0.000E+00
 22       NO    +     OH             =        HNO2                                      9.799E+03     -8.060E+02
 23       HNO2                       =        NO     +      OH                          1.975E-01      0.000E+00
 24       OH    +     HNO2           =        NO2                                       9.770E+03      0.000E+00
 25       HNO2  +     HNO2           =        NO     +      NO2                         1.500E-05      0.000E+00
```

```
THE REACTIONS                                                                 RATE CONSTANT  ACT. ENERGY(K)
26   NO2   +  OH            =      HNO3                                       1.682E+04  -7.130E+02
27   OH    +  HNO3          =      NO3                                        2.179E+02  -1.000E+03
28   HO2   +  NO            =      OH   +      NO2                            1.227E+04  -2.400E+02
29   HO2   +  NO2           =      PNA                                        2.025E+03  -7.490E+02
30   PNA                    =      HO2  +      NO2                            5.115E+00   1.012E+04
31   OH    +  PNA           =      NO2                                        6.833E+03  -3.800E+02
32   HO2   +  HO2           =      H2O2                                       4.144E+03  -1.150E+03
33   HO2   +  HO2   +  H2O  =      H2O2                                       2.181E-01  -5.800E+03
34   H2O2                   =    2 OH                                         1.890E-01   0.000E+00
35   OH    +  H2O2          =      HO2                                        2.520E+03   1.870E+02
36   OH    +  CO            =      HO2                                        3.220E+02   0.000E+00
37   FORM  +  OH            =      HO2  +      CO                             1.500E+04   0.000E+00
38   FORM                   =    2 HO2  +      CO                             1.000E+00   0.000E+00
39   FORM                   =      CO                                         1.000E+00   0.000E+00
40   FORM  +  O             =      OH   +      HO2  +      CO                 2.370E+02   1.550E+03
41   FORM  +  NO3           =      HNO3 +      HO2  +      CO                 9.300E-01   0.000E+00
42   ALD2  +  O             =      C2O3 +      OH                             6.360E+02   9.860E+02
43   ALD2  +  OH            =      C2O3                                       2.400E+04  -2.500E+02
44   ALD2  +  NO3           =      C2O3 +      HNO3                           3.700E+00   0.000E+00
45   ALD2                   =      FORM +    2 HO2  +      CO   +      XO2    1.000E+00   0.000E+00
46   C2O3  +  NO            =      FORM +      NO2  +      HO2  +      XO2    1.831E+04  -2.500E+02
47   C2O3  +  NO2           =      PAN                                        1.223E+04  -5.500E+03
48   PAN                    =      C2O3 +      NO2                            2.220E-02   1.400E+04
49   C2O3  +  C2O3          =    2 FORM +    2 XO2  +    2 HO2                3.700E+03   0.000E+00
50   C2O3  +  HO2           = 0.79 FORM + 0.79 XO2  + 0.79 HO2  + 0.79 OH     9.600E-03   0.000E+00
```

```
THE REACTIONS                                                                                  RATE CONSTANT  ACT. ENERGY(K)
  51        OH                         =        FORM  +      X02   +      H02                    2.100E+01      1.710E+03
  52        PAR   +      OH            =   0.87 X02   + 0.13 X02N  + 0.11 H02   + 0.11 ALD2      1.203E+03      0.000E+00
                                         - 0.11 PAR   + 0.76 ROR
  53        ROR                        =   0.96 X02   +  1.1 ALD2  + 0.94 H02   -  2.1 PAR       1.371E+05      8.000E+03
                                         + 0.04 X02N  + 0.02 ROR
  54        ROR                        =        H02                                              9.545E+04      0.000E+00
  55        ROR   +      NO2           =                                                         2.200E+04      0.000E+00
  56        O     +      OLE           =   0.63 ALD2  + 0.38 H02   + 0.28 X02   +  0.3 CO        5.920E+03      3.240E+02
                                         +  0.2 FORM  + 0.02 X02N  + 0.22 PAR   +  0.2 OH
  57        OH    +      OLE           =        FORM  +      ALD2  -      PAR   +      X02       4.200E+04     -5.040E+02
                                         +      H02
  58        O3    +      OLE           =    0.5 ALD2  + 0.74 FORM  + 0.22 X02   +  0.1 OH        1.800E-02      2.105E+03
                                         + 0.33 CO    + 0.44 H02   -      PAR
  59        NO3   +      OLE           =   0.91 X02   +      FORM  + 0.09 X02N  +      ALD2      1.135E+01      0.000E+00
                                         +      NO2   -      PAR
  60        O     +      ETH           =        FORM  +  1.7 H02   +      CO    +  0.7 X02       1.080E+03      7.920E+02
                                         +  0.3 OH
  61        OH    +      ETH           =        X02   + 1.56 FORM  + 0.22 ALD2  +      H02       1.192E+04     -4.110E+02
  62        O3    +      ETH           =        FORM  + 0.42 CO    + 0.12 H02                    2.702E-03      2.633E+03
  63        TOL   +      OH            =   0.44 H02   + 0.08 X02   + 0.36 CRES  + 0.56 TO2       9.150E+03     -3.220E+02
  64        TO2   +      NO            =    0.9 NO2   +  0.9 H02   +  0.9 OPEN                   1.200E+04      0.000E+00
  65        TO2                        =        CRES  +      H02                                 2.500E+02      0.000E+00
  66        OH    +      CRES          =    0.4 CRO   +  0.6 X02   +  0.6 H02   +  0.3 OPEN      6.100E+04      0.000E+00
  67        CRES  +      NO3           =        CRO   +      HNO3                                3.250E+04      0.000E+00
  68        CRO   +      NO2           =                                                         2.000E+04      0.000E+00
  69        OPEN                       =        C2O3  +      H02   +      CO                     8.400E+00      0.000E+00
  70        OPEN  +      OH            =        X02   +    2 CO    +    2 H02   +      C2O3      4.400E+04      0.000E+00
                                         +      FORM
```

```
THE REACTIONS                                                                                   RATE CONSTANT  ACT. ENERGY(K)
 71        OPEN  +      O3               =    0.03 ALD2  + 0.62 C2O3   +  0.7 FORM  + 0.03 XO2    1.500E-02       5.000E+02
                                           + 0.69 CO     + 0.08 OH     + 0.76 HO2   +  0.2 MGLY
 72        OH    +      XYL              =     0.7 HO2   +  0.5 XO2    +  0.2 CRES  +  0.8 MGLY   3.620E+04      -1.160E+02
                                           +   1.1 PAR   +  0.3 TO2
 73        OH    +      MGLY             =         XO2   +      C2O3                              2.600E+04       0.000E+00
 74        MGLY                          =         C2O3  +      HO2    +      CO                  8.960E+00       0.000E+00
 75        O     +      ISOP             =     0.6 HO2   +  0.8 ALD2   + 0.55 OLE   +  0.5 XO2    2.700E+04       0.000E+00
                                           +   0.5 CO    + 0.45 ETH    +  0.9 PAR
 76        OH    +      ISOP             =         XO2   +      FORM   + 0.67 HO2   + 0.13 XO2N   1.420E+05       0.000E+00
                                           +       ETH   +  0.4 MGLY   +  0.2 C2O3  +  0.2 ALD2
 77        O3    +      ISOP             =         FORM  +  0.4 ALD2   + 0.55 ETH   +  0.2 MGLY   1.800E-02       0.000E+00
                                           +   0.1 PAR   + 0.06 CO     + 0.44 HO2   +  0.1 OH
 78        NO3   +      ISOP             =         XO2N                                           4.700E+02       0.000E+00
 79        XO2   +      NO               =         NO2                                            1.200E+04       0.000E+00
 80        XO2N  +      NO               =                                                        1.000E+03       0.000E+00
 81        XO2   +      XO2              =                                                        2.000E+03      -1.300E+03
 82        NR                            =         NR                                             1.000E+00       0.000E+00
```

```
                                  THE FOLLOWING PHOTOLYSIS RATE CONSTANTS ARE USED
REACTION  SPECIES                                              ZENITH ANGLE (DEG)
  NO.                   0         10        20        30        40        50        60        70        78        86


   1       NO2      5.89E-01  5.85E-01  5.71E-01  5.47E-01  5.09E-01  4.54E-01  3.74E-01  2.58E-01  1.34E-01  2.42E-02

   8       O3       3.12E-02  3.10E-02  3.03E-02  2.90E-02  2.70E-02  2.40E-02  1.98E-02  1.37E-02  7.11E-03  1.28E-03

   9       O3       2.72E-03  2.62E-03  2.36E-03  1.96E-03  1.46E-03  9.44E-04  4.62E-04  1.39E-04  2.95E-05  3.15E-06

  14       NO3      2.00E+01  1.98E+01  1.94E+01  1.85E+01  1.73E+01  1.54E+01  1.27E+01  8.74E+00  4.55E+00  8.20E-01

  23       HNO2     1.16E-01  1.16E-01  1.13E-01  1.08E-01  1.01E-01  8.96E-02  7.39E-02  5.09E-02  2.65E-02  4.78E-03

  34       H2O2     6.40E-04  6.34E-04  6.12E-04  5.73E-04  5.15E-04  4.36E-04  3.27E-04  1.95E-04  8.79E-05  2.40E-05

  38       FORM     2.18E-03  2.14E-03  2.03E-03  1.86E-03  1.60E-03  1.27E-03  8.73E-04  4.48E-04  1.72E-04  4.28E-05

  39       FORM     3.39E-03  3.35E-03  3.24E-03  3.03E-03  2.72E-03  2.30E-03  1.73E-03  1.03E-03  4.65E-04  1.27E-04

  45       ALD2     3.47E-04  3.38E-04  3.14E-04  2.75E-04  2.22E-04  1.61E-04  9.61E-05  4.07E-05  1.22E-05  2.27E-06

  69       OPEN     1.83E-02  1.80E-02  1.71E-02  1.56E-02  1.34E-02  1.07E-02  7.33E-03  3.76E-03  1.44E-03  3.60E-04

  74       MGLY     1.95E-02  1.92E-02  1.82E-02  1.67E-02  1.43E-02  1.14E-02  7.82E-03  4.01E-03  1.54E-03  3.84E-04
```

```
EXAMPLE 1 - SINGLE CALCULATION


PHOTOLYTIC RATE CONSTANTS CALCULATED FOR

        TEST CITY

LATITUDE      38.629
LONGITUDE     90.206
TIME ZONE     5.0
DATE          6     21    1986
TIME          800   TO    1800      LOCAL DAYLIGHT TIME


DILUTION DETERMINED FROM THE FOLLOWING
INVERSION HEIGHTS      INITIAL   250.     FINAL      1700.
TIMING                 START     800.     STOP       1500.


MIXING HEIGHTS (AT THE BEGINNING OF EACH HOUR)
TIME        800     900     1000    1100    1200    1300    1400    1500

HEIGHT      250.0   503.1   821.2  1119.5  1340.2  1496.2  1610.8  1700.0

REACTIVITY

EMISSIONS       ETH  FRACTION  .037   OLE  FRACTION  .035   ALD2 FRACTION  .052

EMISSIONS       FORM FRACTION  .021   TOL  FRACTION  .089   XYL  FRACTION  .117

EMISSIONS       PAR  FRACTION  .564   ISOP FRACTION  .000   NR   FRACTION  .085

ALOFT           ETH  FRACTION  .034   OLE  FRACTION  .020   ALD2 FRACTION  .037

ALOFT           FORM FRACTION  .070   TOL  FRACTION  .042   XYL  FRACTION  .026

ALOFT           PAR  FRACTION  .498   ISOP FRACTION  .000   NR   FRACTION  .273

NO2/NOX        .250
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TRANSPORTED CONCENTRATIONS
ALOFT              OZONE    .080     HYDROCARBON   .050    NOX      .009 PPM


CONTINUOUS EMISSIONS (EXPRESSED AS FRACTION OF THE INITIAL PRECURSORS)
SPECIES     HOUR          1     2     3     4     5     6     7     8     9    10
                         11

  VOC     FRACTION      .106  .086  .084  .058  .036  .025  .024  .020  .019  .024
                        .013

  NOX     FRACTION      .343  .262  .239  .174  .117  .080  .081  .068  .060  .075
                        .038
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                              EXAMPLE 1 - SINGLE CALCULATION
THE ERROR TOLERANCE IS  3.000E-03

THE TEMPERATURE USED IS  3.030E+02

THE MIXING HEIGHT IS  2.50E+02

THE RATE CONSTANTS USED WERE

   3.248E-01   4.051E+06   2.874E+01   1.375E+04   2.223E+03   2.358E+03   5.418E-02   1.722E-02   2.835E-04   4.155E+05
   3.260E+00   1.053E+02   3.098E+00   1.101E+01   4.355E+04   6.317E-01   1.827E+03   1.900E-06   5.076E+00   1.494E-04
   1.600E-11   9.371E+03   6.416E-02   9.770E+03   1.500E-05   1.617E+04   2.062E+02   1.211E+04   1.943E+03   8.959E+00
   6.691E+03   3.888E+03   1.582E-01   2.708E-04   2.546E+03   3.220E+02   1.500E+04   6.762E-04   1.433E-03   2.582E+02
   9.300E-01   6.717E+02   2.367E+04   3.700E+00   6.830E-05   1.806E+04   9.019E+03   4.820E-02   3.700E+03   9.600E+03
   2.309E+01   1.203E+03   2.135E+05   9.545E+04   2.200E+04   6.027E+03   4.084E+04   2.023E-02   1.135E+01   1.128E+03
   1.165E+04   3.126E-03   8.988E+03   1.200E+04   2.500E+02   6.100E+04   3.250E+04   2.000E+04   5.680E-03   4.400E+04
   1.542E-02   3.597E+04   2.600E+04   6.059E-03   2.700E+04   1.420E+05   1.800E-02   4.700E+02   1.200E+04   1.000E+03
   1.861E+03   1.000E+00
THE PHOTOLYSIS REACTIONS ARE

           1           8           9          14          23          34          38          39          45
          69          74

THE PHOTOLYTIC RATE CONSTANTS ARE
        3.248E-01   1.722E-02   2.835E-04   1.101E+01   6.416E-02   2.708E-04   6.762E-04   1.433E-03   6.830E-05
        5.680E-03   6.059E-03
        TIME     NMOC       NMOC/        NOX          NO2          O3          NO2          PAR
        (LDT )   TOTAL       NOX         TOTAL      FRACTION   (INSTANT)   (INSTANT)   (INSTANT)

        800.    1.00000   10.00000      .10000       .25000      .00000      .02500      .56400

  TIME        NO2         NO          O           O3          NO3         O1D         H2O         OH          HO2         N2O5
INTERVAL      HNO3        HNO2        PNA         H2O2        CO          FORM        ALD2        C2O3        XO2         PAN
              PAR         XO2N        ROR         OLE         ETH         TOL         CRES        TO2         OPEN        CRO
              MGLY        XYL         ISOP        NR

8.000E+02   2.500E-02   7.500E-02   0.000E+00   0.000E+00   0.000E+00   0.000E+00   2.000E+04   0.000E+00   0.000E+00   0.000E+00
1.000E-10   0.000E+00   0.000E+00   0.000E+00   0.000E+00   1.200E+00   2.100E-02   2.600E-02   0.000E+00   0.000E+00   0.000E+00
            5.640E-01   0.000E+00   0.000E+00   1.750E-02   1.850E-02   1.271E-02   0.000E+00   0.000E+00   0.000E+00   0.000E+00
            0.000E+00   1.462E-02   0.000E+00   8.500E-02

NET RATES  -8.296E-03   7.700E-03   8.121E-03   1.027E-03   0.000E+00   0.000E+00  -6.000E-10   0.000E+00   3.195E-05   0.000E+00
            0.000E+00   1.200E-09   0.000E+00   0.000E+00  -8.937E-03  -2.300E-04  -2.776E-04   0.000E+00   1.776E-06   0.000E+00
           -5.922E-03   0.000E+00   0.000E+00  -1.873E-04  -1.938E-04  -1.369E-04   0.000E+00   0.000E+00   0.000E+00   0.000E+00
            0.000E+00  -1.598E-04   0.000E+00  -7.655E-04

THE REACTION RATES ARE
     8.12E-03    0.00E+00    0.00E+00    0.00E+00    0.00E+00    0.00E+00    0.00E+00    0.00E+00    0.00E+00    0.00E+00
     0.00E+00    0.00E+00    0.00E+00    0.00E+00    0.00E+00    0.00E+00    0.00E+00    0.00E+00    0.00E+00    8.41E-07
     6.00E-10    0.00E+00    0.00E+00    0.00E+00    0.00E+00    0.00E+00    0.00E+00    0.00E+00    0.00E+00    0.00E+00
     0.00E+00    0.00E+00    0.00E+00    0.00E+00    0.00E+00    0.00E+00    0.00E+00    1.42E-05    3.01E-05    0.00E+00
     0.00E+00    0.00E+00    0.00E+00    0.00E+00    1.78E-06    0.00E+00    0.00E+00    0.00E+00    0.00E+00    0.00E+00
     0.00E+00    0.00E+00    0.00E+00    0.00E+00    0.00E+00    0.00E+00    0.00E+00    0.00E+00    0.00E+00    0.00E+00
     0.00E+00    0.00E+00    0.00E+00    0.00E+00    0.00E+00    0.00E+00    0.00E+00    0.00E+00    0.00E+00    0.00E+00
     0.00E+00    0.00E+00    0.00E+00    0.00E+00    0.00E+00    0.00E+00    0.00E+00    0.00E+00    0.00E+00    0.00E+00
     0.00E+00    8.50E-02                                                                                         0.00E+00

THE PHOTOLYTIC RATE CONSTANTS ARE
     3.248E-01   1.722E-02   2.835E-04   1.101E+01   6.416E-02   2.708E-04   6.762E-04   1.433E-03   6.830E-05
     5.680E-03   6.059E-03


THE CURRENT MIXING HEIGHT IS      250.00

THE CURRENT TEMPERATURE IS        303.00

THE CURRENT ZENITH ANGLE IS        64.75
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          TIME     NMOC      NMOC/      NOX        NO2          O3          NO2         PAR
         (LDT )    TOTAL      NOX      TOTAL     FRACTION   (INSTANT)   (INSTANT)   (INSTANT)

          900.    .56332    8.13658    .06923     .62694      .02527      .04341      .31967

   TIME       NO2         NO          O           O3          NO3         O1D         H2O         OH          HO2         N2O5
 INTERVAL     HNO3        HNO2        PNA         H2O2        CO          FORM        ALD2        C2O3        XO2         PAN
              PAR         XO2N        ROR         OLE         ETH         TOL         CRES        TO2         OPEN        CRO
              MGLY        XYL         ISOP        NR

 9.000E+02   4.341E-02   2.583E-02   4.773E-09   2.527E-02   5.211E-08   4.119E-11   2.000E+04   6.386E-08   5.523E-07   8.016E-07
 9.182E+00   1.414E-03   1.815E-04   5.183E-06   4.183E-08   8.496E-01   1.360E-02   1.559E-02   5.003E-08   3.320E-07   2.426E-04
             3.197E-01   1.439E-07   6.105E-11   8.676E-03   1.023E-02   6.960E-03   2.954E-04   1.304E-08   1.517E-04   1.107E-09
             4.737E-04   7.347E-03   0.000E+00   5.356E-02

 NET RATES  -8.855E-06  -3.994E-04  -3.147E-07   4.570E-04  -5.316E-08   2.852E-09  -2.717E-06   2.727E-08  -3.341E-08   2.562E-08
             3.133E-05  -1.936E-06   8.093E-08   1.712E-09  -3.421E-03  -7.529E-05  -1.072E-04  -4.765E-09  -2.163E-08   5.479E-06
            -2.544E-03   9.509E-10   5.308E-09  -9.467E-05  -8.702E-05  -6.008E-05   3.489E-06  -6.389E-10   5.230E-07  -1.120E-10
             3.135E-06  -7.665E-05   0.000E+00  -3.292E-04

 THE REACTION RATES ARE
       1.87E-02    1.93E-02    1.88E-02    2.85E-06    4.60E-07    2.91E-07    5.94E-05    5.78E-04    1.98E-05    1.71E-05
       2.69E-06    1.70E-07    4.32E-08    7.63E-07    5.86E-05    1.43E-09    4.13E-06    3.05E-08    4.07E-06    9.97E-08
       3.59E-10    1.55E-05    1.55E-05    1.13E-07    4.94E-13    4.48E-05    1.86E-08    1.73E-04    4.66E-05    4.64E-05
       2.21E-09    1.19E-09    9.65E-10    1.69E-11    6.80E-12    1.75E-05    1.30E-05    1.57E-05    2.91E-05    1.68E-08
       6.59E-10    5.00E-08    2.36E-05    3.01E-09    2.19E-06    2.33E-05    1.96E-05    1.17E-05    9.26E-12    2.65E-10
       1.47E-06    2.46E-05    1.30E-05    5.83E-06    5.83E-08    2.50E-07    2.26E-05    4.43E-06    5.13E-09    5.51E-08
       7.61E-06    8.08E-07    4.00E-06    4.04E-06    3.26E-06    1.15E-06    5.00E-07    9.61E-07    1.47E-06    4.26E-07
       5.91E-08    1.69E-05    7.87E-07    4.89E-06    0.00E+00    0.00E+00    0.00E+00    0.00E+00    1.03E-04    3.72E-06
       2.05E-10    5.36E-02

 THE PHOTOLYTIC RATE CONSTANTS ARE
         4.318E-01    2.288E-02    7.838E-04    1.464E+01    8.527E-02    4.039E-04    1.151E-03    2.137E-03    1.406E-04
         9.670E-03    1.031E-02


 THE CURRENT MIXING HEIGHT IS       503.11

 THE CURRENT TEMPERATURE IS         303.00

 THE CURRENT ZENITH ANGLE IS         53.12
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   TIME      NMOC       NMOC/        NOX         NO2          O3          NO2         PAR
  (LDT )     TOTAL       NOX         TOTAL     FRACTION   (INSTANT)   (INSTANT)   (INSTANT)

  1000.     .37836     7.51671      .05034      .74531      .05041      .03752      .21701

  TIME        NO2         NO          O           O3          NO3         O1D         H2O         OH          HO2         N2O5
INTERVAL      HNO3        HNO2        PNA         H2O2        CO          FORM        ALD2        C2O3        XO2         PAN
              PAR         XO2N        ROR         OLE         ETH         TOL         CRES        TO2         OPEN        CRO
              MGLY        XYL         ISOP        NR

 1.000E+03   3.752E-02   1.282E-02   5.001E-09   5.041E-02   1.745E-07   1.454E-10   2.000E+04   1.031E-07   1.247E-06   2.332E-06
 1.569E+01   3.566E-03   1.193E-04   1.013E-05   3.118E-07   7.166E-01   1.064E-02   1.131E-02   1.211E-07   7.198E-07   6.190E-04
             2.170E-01   3.174E-07   6.696E-11   4.714E-03   6.658E-03   4.516E-03   4.253E-04   1.731E-08   1.432E-04   4.640E-09
             5.370E-04   4.177E-03   0.000E+00   4.031E-02

NET RATES   -1.119E-04  -1.162E-04  -2.008E-07   3.558E-04  -1.007E-08   8.613E-10  -9.577E-06   2.377E-08   1.563E-09   1.955E-08
             4.174E-05  -3.519E-07   7.744E-08   8.688E-09  -1.364E-03  -2.861E-05  -4.400E-05   4.625E-10  -2.475E-10   7.082E-06
            -1.081E-03   3.271E-09  -1.936E-10  -4.482E-05  -3.910E-05  -2.628E-05   1.064E-06  -1.069E-10  -3.695E-07   4.272E-10
            -2.526E-08  -3.544E-05   0.000E+00  -1.377E-04

THE REACTION RATES ARE
      1.89E-02    2.03E-02    1.86E-02    2.58E-06    4.17E-07    1.51E-07    1.02E-04    1.34E-03    6.99E-05    6.04E-05
      9.48E-06    5.47E-07    1.95E-07    2.97E-06    9.74E-05    4.14E-09    1.20E-05    8.86E-08    1.18E-05    2.46E-08
      1.54E-10    1.24E-05    1.18E-05    1.20E-07    2.13E-13    6.25E-05    7.58E-08    1.94E-04    9.09E-05    9.07E-05
      6.99E-09    6.05E-09    4.92E-09    1.58E-10    8.19E-11    2.38E-05    1.65E-05    1.66E-05    2.85E-05    1.37E-08
      1.73E-09    3.80E-08    2.76E-05    7.30E-09    2.41E-06    2.80E-05    4.10E-05    2.98E-05    5.42E-11    1.45E-09
      2.38E-06    2.69E-05    1.43E-05    6.39E-06    5.53E-08    1.42E-07    1.99E-05    4.81E-06    9.34E-09    3.76E-08
      8.00E-06    1.05E-06    4.19E-06    2.66E-06    4.33E-06    2.67E-06    2.41E-06    3.48E-06    1.87E-06    6.49E-07
      1.11E-07    1.55E-05    1.44E-06    7.49E-06    0.00E+00    0.00E+00    0.00E+00    0.00E+00    1.11E-04    4.07E-06
      9.64E-10    4.03E-02

THE PHOTOLYTIC RATE CONSTANTS ARE
         5.025E-01   2.663E-02   1.387E-03   1.704E+01   9.925E-02   5.053E-04   1.556E-03   2.673E-03   2.133E-04
         1.307E-02   1.394E-02


THE CURRENT MIXING HEIGHT IS      821.23

THE CURRENT TEMPERATURE IS        303.00

THE CURRENT ZENITH ANGLE IS        41.43
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          TIME       NMOC        NMOC/        NOX         NO2          O3          NO2          PAR
         (LDT )      TOTAL        NOX        TOTAL      FRACTION    (INSTANT)   (INSTANT)   (INSTANT)

         1100.      .29574      7.49239      .03947      .79029      .06994      .03119      .17254

   TIME          NO2         NO          O           O3          NO3         O1D         H2O         OH          HO2         N2O5
 INTERVAL        HNO3        HNO2        PNA         H2O2        CO          FORM        ALD2        C2O3        XO2         PAN
                 PAR         XO2N        ROR         OLE         ETH         TOL         CRES        TO2         OPEN        CRO
                 MGLY        XYL         ISOP        NR

 1.100E+03    3.119E-02   8.278E-03   4.740E-09   6.994E-02   3.014E-07   2.851E-10   2.000E+04   1.609E-07   2.297E-06   3.352E-06
 1.569E+01    6.576E-03   1.107E-04   1.551E-05   1.371E-06   6.617E-01   9.620E-03   9.522E-03   2.401E-07   1.306E-06   1.112E-03
              1.725E-01   6.093E-07   8.312E-11   2.704E-03   4.948E-03   3.394E-03   4.407E-04   2.072E-08   1.234E-04   9.692E-09
              5.122E-04   2.585E-03   0.000E+00   3.479E-02

NET RATES    -9.876E-05  -5.526E-05   9.341E-07   3.114E-04  -8.667E-09  -1.371E-08  -1.873E-05  -2.388E-08  -9.861E-09   2.375E-08
              5.996E-05  -7.024E-08   1.542E-07   3.054E-08  -5.760E-04  -9.165E-06  -2.060E-05   7.946E-09   3.075E-08   9.622E-06
             -5.069E-04   7.621E-09  -2.843E-09  -2.570E-05  -2.151E-05  -1.363E-05  -4.171E-07   1.992E-10  -2.631E-07   4.475E-10
             -6.622E-07  -2.058E-05   0.000E+00  -6.012E-05

THE REACTION RATES ARE
       1.71E-02    1.92E-02    1.66E-02    2.03E-06    3.29E-07    9.25E-08    1.18E-04    2.03E-03    1.37E-04    1.18E-04
       1.86E-05    1.19E-06    4.98E-07    5.59E-06    1.09E-04    5.94E-09    1.72E-05    1.27E-07    1.70E-05    1.02E-08
       8.26E-11    1.25E-05    1.19E-05    1.74E-07    1.84E-13    8.12E-05    2.18E-07    2.30E-04    1.39E-04    1.39E-04
       1.67E-08    2.05E-08    1.67E-08    7.85E-10    5.62E-10    3.43E-05    2.32E-05    1.79E-05    2.91E-05    1.18E-08
       2.70E-09    3.03E-08    3.63E-05    1.06E-08    2.61E-06    3.59E-05    6.75E-05    5.36E-05    2.13E-10    5.29E-09
       3.71E-06    3.34E-05    1.77E-05    7.93E-06    5.70E-08    7.73E-08    1.78E-05    3.83E-06    9.25E-09    2.65E-08
       9.28E-06    1.08E-06    4.91E-06    2.06E-06    5.18E-06    4.33E-06    4.32E-06    6.05E-06    1.93E-06    8.74E-07
       1.33E-07    1.50E-05    2.14E-06    8.53E-06    0.00E+00    0.00E+00    0.00E+00    0.00E+00    1.30E-04    5.04E-06
       3.17E-09    3.48E-02

THE PHOTOLYTIC RATE CONSTANTS ARE
        5.467E-01    2.898E-02    1.959E-03    1.853E+01    1.080E-01    5.723E-04    1.858E-03    3.028E-03    2.741E-04
        1.560E-02    1.664E-02


THE CURRENT MIXING HEIGHT IS     1119.47

THE CURRENT TEMPERATURE IS        303.00

THE CURRENT ZENITH ANGLE IS        30.10
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           TIME     NMOC       NMOC/       NOX        NO2        O3         NO2        PAR
           (LDT )   TOTAL      NOX         TOTAL      FRACTION   (INSTANT)  (INSTANT)  (INSTANT)

           1200.    .25023     8.10484     .03087     .82299     .08911     .02541     .14952

 TIME          NO2         NO          O           O3          NO3         O1D         H2O         OH          HO2         N2O5
 INTERVAL      HNO3        HNO2        PNA         H2O2        CO          FORM        ALD2        C2O3        XO2         PAN
               PAR         XO2N        ROR         OLE         ETH         TOL         CRES        TO2         OPEN        CRO
               MGLY        XYL         ISOP        NR

  1.200E+03    2.541E-02   5.465E-03   4.293E-09   8.911E-02   4.569E-07   4.363E-10   2.000E+04   2.354E-07   4.091E-06   4.143E-06
  1.892E+01    1.072E-02   1.042E-04   2.252E-05   4.924E-06   6.380E-01   9.268E-03   8.480E-03   4.489E-07   2.292E-06   1.784E-03
               1.495E-01   1.169E-06   1.054E-10   1.466E-03   3.863E-03   2.727E-03   3.795E-04   2.281E-08   1.065E-04   1.538E-08
               4.509E-04   1.562E-03   0.000E+00   3.224E-02

 NET RATES    -1.005E-04  -3.912E-05   6.024E-08   3.378E-04   1.295E-08  -3.365E-10  -2.865E-05  -5.768E-08   8.339E-08   1.347E-08
               7.757E-05  -1.716E-07   1.456E-07   1.008E-07  -2.668E-04  -4.484E-06  -1.637E-05   1.297E-08   4.600E-08   1.282E-05
              -3.021E-04   1.493E-08  -8.868E-10  -1.651E-05  -1.597E-05  -9.530E-06  -1.529E-06  -3.179E-10  -3.298E-07   3.656E-10
              -1.393E-06  -1.435E-05   0.000E+00  -3.055E-05

 THE REACTION RATES ARE
        1.45E-02    1.74E-02    1.40E-02    1.50E-06    2.42E-07    5.53E-08    1.23E-04    2.70E-03    2.10E-04    1.81E-04
        2.84E-05    2.21E-06    1.13E-06    8.84E-06    1.09E-04    7.33E-09    2.12E-05    1.57E-07    2.10E-05    4.46E-09
        4.44E-11    1.21E-05    1.17E-05    2.40E-07    1.63E-13    9.67E-05    5.20E-07    2.71E-04    2.02E-04    2.02E-04
        3.55E-08    6.51E-08    5.29E-08    3.01E-09    2.95E-09    4.84E-05    3.27E-05    1.88E-05    3.00E-05    1.03E-08
        3.94E-09    2.45E-08    4.72E-05    1.43E-08    2.66E-06    4.43E-05    1.03E-04    8.60E-05    7.46E-10    1.76E-08
        5.43E-06    4.23E-05    2.25E-05    1.01E-05    5.89E-08    3.79E-08    1.41E-05    2.64E-06    7.60E-09    1.87E-08
        1.06E-05    1.08E-06    5.77E-06    1.50E-06    5.70E-06    5.45E-06    5.63E-06    7.81E-06    1.82E-06    1.10E-06
        1.46E-07    1.32E-05    2.76E-06    8.21E-06    0.00E+00    0.00E+00    0.00E+00    0.00E+00    1.50E-04    6.39E-06
        9.78E-09    3.22E-02

 THE PHOTOLYTIC RATE CONSTANTS ARE
        5.710E-01   3.026E-02   2.353E-03   1.936E+01   1.128E-01   6.117E-04   2.031E-03   3.236E-03   3.136E-04
        1.706E-02   1.820E-02


 THE CURRENT MIXING HEIGHT IS     1340.22

 THE CURRENT TEMPERATURE IS        303.00

 THE CURRENT ZENITH ANGLE IS        20.18
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  TIME      NMOC        NMOC/         NOX         NO2          O3          NO2          PAR
 (LDT )     TOTAL        NOX         TOTAL      FRACTION   (INSTANT)    (INSTANT)    (INSTANT)

 1300.     .21774      9.67447      .02251      .85293      .11076       .01920       .13376

  TIME         NO2         NO          O           O3          NO3         O1D         H2O         OH          HO2         N2O5
INTERVAL       HNO3        HNO2        PNA         H2O2        CO          FORM        ALD2        C2O3        XO2         PAN
               PAR         XO2N        ROR         OLE         ETH         TOL         CRES        TO2         OPEN        CRO
               MGLY        XYL         ISOP        NR

 1.300E+03   1.920E-02   3.310E-03   3.646E-09   1.108E-01   6.728E-07   5.773E-10   2.000E+04   3.346E-07   7.756E-06   4.613E-06
 2.000E+01   1.569E-02   8.974E-05   3.227E-05   1.733E-05   6.261E-01   8.938E-03   7.434E-03   8.537E-07   4.272E-06   2.652E-03
             1.338E-01   2.445E-06   1.341E-10   6.842E-04   2.965E-03   2.197E-03   2.744E-04   2.319E-08   8.305E-05   2.146E-08
             3.476E-04   8.364E-04   0.000E+00   3.081E-02

NET RATES   -1.079E-04  -3.052E-05  -1.137E-08   3.874E-04   1.239E-08  -3.947E-09  -3.801E-05  -4.971E-07   7.078E-07   3.050E-09
             8.616E-05  -3.119E-07   2.139E-09   3.732E-07  -1.453E-04  -7.212E-06  -1.862E-05   1.353E-07   2.643E-07   1.610E-05
            -2.322E-04   4.966E-08   1.446E-09  -9.713E-06  -1.415E-05  -8.325E-06  -1.812E-06   1.115E-09  -4.382E-07   1.907E-09
            -1.976E-06  -9.833E-06   0.000E+00  -1.805E-05

THE REACTION RATES ARE
      1.11E-02    1.48E-02    1.05E-02    9.63E-07    1.56E-07    2.85E-08    1.15E-04    3.40E-03    2.78E-04    2.40E-04
      3.76E-05    3.90E-06    2.66E-06    1.32E-05    9.70E-05    8.16E-09    2.36E-05    1.75E-07    2.34E-05    1.64E-09
      2.03E-11    1.04E-05    1.03E-05    2.93E-07    1.21E-13    1.04E-04    1.08E-06    3.11E-04    2.89E-04    2.89E-04
      7.23E-08    2.34E-07    1.90E-07    1.08E-08    1.48E-08    6.75E-05    4.49E-05    1.87E-05    2.95E-05    8.42E-09
      5.59E-09    1.82E-08    5.89E-05    1.85E-08    2.44E-06    5.10E-05    1.48E-04    1.28E-04    2.70E-09    6.36E-08
      7.72E-06    5.38E-05    2.86E-05    1.28E-05    5.66E-08    1.50E-08    9.35E-06    1.53E-06    5.23E-09    1.22E-08
      1.16E-05    1.03E-06    6.61E-06    9.21E-07    5.80E-06    5.60E-06    6.00E-06    8.24E-06    1.46E-06    1.22E-06
      1.42E-07    1.01E-05    3.02E-06    6.52E-06    0.00E+00    0.00E+00    0.00E+00    0.00E+00    1.70E-04    8.09E-06
      3.40E-08    3.08E-02

THE PHOTOLYTIC RATE CONSTANTS ARE
         5.793E-01   3.070E-02   2.506E-03   1.964E+01   1.144E-01   6.247E-04   2.094E-03   3.305E-03   3.278E-04
         1.759E-02   1.876E-02


THE CURRENT MIXING HEIGHT IS     1496.21

THE CURRENT TEMPERATURE IS        303.00

THE CURRENT ZENITH ANGLE IS        15.19
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    TIME      NMOC       NMOC/        NOX         NO2         O3          NO2         PAR
   (LDT )     TOTAL       NOX         TOTAL      FRACTION   (INSTANT)   (INSTANT)   (INSTANT)

   1400.     .19088    13.26779     .01439      .88188      .13559      .01269      .12036

  TIME         NO2          NO           O           O3          NO3         O1D         H2O          OH          HO2         N2O5
INTERVAL       HNO3         HNO2         PNA         H2O2        CO          FORM        ALD2         C2O3        XO2         PAN
               PAR          XO2N         ROR         OLE         ETH         TOL         CRES         TO2         OPEN        CRO
               MGLY         XYL          ISOP        NR

 1.400E+03   1.269E-02   1.699E-03   2.880E-09   1.356E-01   9.588E-07   6.702E-10   2.000E+04   4.675E-07   1.695E-05   4.344E-06
 2.000E+01   2.071E-02   6.641E-05   4.647E-05   7.121E-05   6.189E-01   8.337E-03   6.249E-03   1.776E-06   9.224E-06   3.723E-03
             1.204E-01   5.966E-06   1.686E-10   2.652E-04   2.148E-03   1.708E-03   1.759E-04   2.174E-08   5.669E-05   2.956E-08
             2.240E-04   3.729E-04   0.000E+00   2.991E-02

NET RATES   -1.130E-04  -1.398E-05   8.887E-08   4.441E-04   3.259E-08   3.929E-10  -4.477E-05   1.833E-07  -1.165E-06   6.534E-09
             7.831E-05  -4.334E-07   1.216E-06   1.823E-06  -1.035E-04  -1.267E-05  -1.997E-05  -4.211E-07   1.041E-07   1.995E-05
            -2.127E-04   9.587E-08   3.185E-08  -4.446E-06  -1.279E-05  -7.830E-06  -1.405E-06   2.321E-08  -4.114E-07  -1.381E-08
            -2.010E-06  -5.562E-06   0.000E+00  -1.144E-05

THE REACTION RATES ARE
     7.26E-03    1.17E-02    6.62E-03    5.02E-07    8.12E-08    1.15E-08    9.32E-05    4.11E-03    3.22E-04    2.78E-04
     4.37E-05    6.68E-06    7.12E-06    1.86E-05    7.10E-05    7.68E-09    2.22E-05    1.65E-07    2.20E-05    4.32E-10
     6.90E-12    7.44E-06    7.51E-06    3.03E-07    6.62E-14    9.59E-05    2.00E-06    3.49E-04    4.18E-04    4.16E-04
     1.45E-07    1.12E-06    9.09E-07    4.37E-08    8.48E-08    9.32E-05    5.85E-05    1.70E-05    2.71E-05    6.20E-09
     7.43E-09    1.21E-08    6.92E-05    2.22E-08    1.97E-06    5.45E-05    2.03E-04    1.79E-04    1.17E-08    2.89E-07
     1.08E-05    6.77E-05    3.60E-05    1.61E-05    4.71E-08    4.60E-09    5.06E-06    7.27E-07    2.89E-09    6.98E-09
     1.17E-05    9.11E-07    7.18E-06    4.43E-07    5.43E-06    5.02E-06    5.48E-06    7.50E-06    9.72E-07    1.17E-06
     1.19E-07    6.27E-06    2.72E-06    4.10E-06    0.00E+00    0.00E+00    0.00E+00    0.00E+00    1.88E-04    1.01E-05
     1.58E-07    2.99E-02

THE PHOTOLYTIC RATE CONSTANTS ARE
       5.722E-01   3.033E-02   2.376E-03   1.940E+01   1.130E-01   6.137E-04   2.041E-03   3.247E-03   3.158E-04
       1.714E-02   1.828E-02


THE CURRENT MIXING HEIGHT IS     1610.77

THE CURRENT TEMPERATURE IS        303.00

THE CURRENT ZENITH ANGLE IS        19.50
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        TIME     NMOC        NMOC/        NOX          NO2          O3         NO2         PAR
       (LDT )    TOTAL        NOX         TOTAL      FRACTION   (INSTANT)   (INSTANT)   (INSTANT)

       1500.     .16816    21.30511      .00789       .90871      .16166      .00717      .10792

  TIME          NO2         NO          O           O3          NO3         O1D         H2O         OH          HO2         N2O5
 INTERVAL       HNO3        HNO2        PNA         H2O2        CO          FORM        ALD2        C2O3        XO2         PAN
                PAR         XO2N        ROR         OLE         ETH         TOL         CRES        TO2         OPEN        CRO
                MGLY        XYL         ISOP        NR

 1.500E+03   7.173E-03   7.206E-04   2.209E-09   1.617E-01   1.226E-06   6.726E-10   2.000E+04   5.740E-07   3.835E-05   3.146E-06
 2.201E+00   2.462E-02   3.791E-05   5.962E-05   3.558E-04   6.130E-01   7.453E-03   5.130E-03   3.982E-06   2.173E-05   4.897E-03
             1.079E-01   1.533E-05   1.858E-10   1.018E-04   1.456E-03   1.269E-03   1.092E-04   1.771E-08   3.556E-05   4.099E-08
             1.187E-04   1.478E-04   0.000E+00   2.935E-02

 NET RATES  -7.582E-05  -1.154E-05  -6.874E-10   4.117E-04   2.955E-09  -2.547E-11  -4.863E-05   1.281E-09   4.397E-07  -2.632E-08
             4.890E-05  -4.794E-07   6.464E-08   9.368E-06  -9.503E-05  -1.558E-05  -1.654E-05   5.250E-08   2.831E-07   1.770E-05
            -2.004E-04   2.191E-07   2.712E-12  -1.469E-06  -9.962E-06  -6.625E-06  -8.658E-07  -8.566E-11  -2.905E-07   1.951E-10
            -1.402E-06  -2.255E-06   0.000E+00  -7.793E-06

 THE REACTION RATES ARE
        3.94E-03    8.95E-03    3.35E-03    2.18E-07    3.52E-08    3.75E-09    6.28E-05    4.71E-03    3.23E-04    2.79E-04
        4.39E-05    9.78E-06    1.92E-05    2.28E-05    3.85E-05    5.55E-09    1.61E-05    1.20E-07    1.60E-05    7.76E-11
        1.65E-12    3.88E-06    4.11E-06    2.13E-07    2.16E-14    6.66E-05    2.91E-06    3.35E-04    5.34E-04    5.34E-04
        2.29E-07    5.72E-06    4.65E-06    2.05E-07    5.20E-07    1.13E-04    6.42E-05    1.40E-05    2.27E-05    4.25E-09
        8.49E-09    7.61E-09    6.97E-05    2.33E-08    1.43E-06    5.18E-05    2.58E-04    2.36E-04    5.87E-08    1.47E-06
        1.33E-05    7.45E-05    3.97E-05    1.77E-05    2.93E-08    1.36E-09    2.39E-06    3.33E-07    1.42E-09    3.63E-09
        8.87E-08    3.05E-06    1.77E-06    2.00E-06    0.00E+00    0.00E+00    0.00E+00    0.00E+00    1.88E-04    1.10E-05
        8.79E-07    2.94E-02

 THE PHOTOLYTIC RATE CONSTANTS ARE
           5.494E-01    2.912E-02    2.000E-03    1.862E+01    1.085E-01    5.766E-04    1.877E-03    3.051E-03    2.783E-04
           1.577E-02    1.682E-02


 THE CURRENT MIXING HEIGHT IS     1700.00

 THE CURRENT TEMPERATURE IS        303.00

 THE CURRENT ZENITH ANGLE IS        29.20
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      TIME      NMOC       NMOC/        NOX        NO2         O3         NO2        PAR
     (LDT )     TOTAL       NOX        TOTAL     FRACTION  (INSTANT)  (INSTANT)  (INSTANT)

     1600.     .15517    36.42352     .00426     .92945     .18534     .00396     .10035

  TIME          NO2         NO          O          O3         NO3        O1D        H2O         OH         HO2        N2O5
  INTERVAL      HNO3        HNO2        PNA        H2O2       CO         FORM       ALD2        C2O3       XO2        PAN
                PAR         XO2N        ROR        OLE        ETH        TOL        CRES        TO2        OPEN       CRO
                MGLY        XYL         ISOP       NR

  1.600E+03   3.960E-03   3.005E-04   1.787E-09   1.853E-01   1.304E-06   5.540E-10   2.000E+04   4.850E-07   5.919E-05   1.848E-06
  1.370E+01   2.749E-02   1.525E-05   5.084E-05   1.362E-03   6.121E-01   6.800E-03   4.472E-03   7.925E-06   3.994E-05   5.751E-03
              1.003E-01   2.894E-05   1.460E-10   4.761E-05   1.006E-03   9.767E-04   6.954E-05   1.086E-08   2.214E-05   4.761E-08
              6.022E-05   7.065E-05   0.000E+00   2.956E-02

  NET RATES  -2.988E-05  -3.640E-06  -2.414E-08   3.067E-04   1.737E-09   1.644E-09  -4.727E-05   3.188E-08   1.031E-07  -1.404E-08
              3.142E-05  -2.339E-07  -2.732E-07   2.233E-05  -1.349E-05  -7.410E-06  -8.086E-06   6.225E-09   1.907E-07   5.791E-06
             -1.033E-04   1.599E-07   1.500E-10  -2.874E-07  -5.387E-06  -3.651E-06  -5.103E-07  -7.532E-11  -1.780E-07  -3.106E-10
             -6.159E-07  -5.343E-07   0.000E+00   4.059E-06

  THE REACTION RATES ARE
      2.01E-03    7.24E-03    1.60E-03    9.73E-08    1.57E-08    1.27E-09    3.98E-05    4.98E-03    2.66E-04    2.30E-04
      3.61E-05    9.47E-06    3.40E-05    2.24E-05    1.71E-05    3.26E-09    9.43E-06    7.02E-08    9.38E-06    1.35E-11
      3.81E-13    1.37E-06    1.53E-06    7.23E-08    3.49E-15    3.10E-05    2.75E-06    2.15E-04    4.55E-04    4.55E-04
      1.65E-07    1.36E-05    1.11E-05    6.97E-07    1.68E-06    9.56E-05    4.95E-05    1.08E-05    1.84E-05    3.14E-09
      8.25E-09    5.37E-09    5.13E-05    2.16E-08    9.79E-07    4.30E-05    2.83E-04    2.77E-04    2.32E-07    4.50E-06
      1.12E-05    5.85E-05    3.12E-05    1.39E-05    1.27E-08    5.13E-10    9.43E-07    1.78E-07    7.05E-10    2.03E-09
      5.68E-06    5.83E-07    4.26E-06    3.92E-08    2.72E-06    2.06E-06    2.95E-06    3.77E-06    2.95E-07    4.72E-07
      6.33E-08    1.23E-06    7.59E-07    8.55E-07    0.00E+00    0.00E+00    0.00E+00    0.00E+00    1.44E-04    8.70E-06
      2.97E-06    2.96E-02

  THE PHOTOLYTIC RATE CONSTANTS ARE
      5.071E-01   2.688E-02   1.437E-03   1.719E+01   1.002E-01   5.118E-04   1.585E-03   2.708E-03   2.188E-04
      1.331E-02   1.420E-02


  THE CURRENT MIXING HEIGHT IS     1701.34

  THE CURRENT TEMPERATURE IS        303.00

  THE CURRENT ZENITH ANGLE IS        40.48
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        TIME      NMOC        NMOC/         NOX          NO2         O3          NO2         PAR
       (LDT )     TOTAL        NOX         TOTAL       FRACTION   (INSTANT)   (INSTANT)   (INSTANT)

       1700.     .14790     45.61844      .00324       .94186      .19954      .00305      .09550

   TIME          NO2         NO          O           O3          NO3         O1D         H2O         OH          HO2         N2O5
 INTERVAL        HNO3        HNO2        PNA         H2O2        CO          FORM        ALD2        C2O3        XO2         PAN
                 PAR         XO2N        ROR         OLE         ETH         TOL         CRES        TO2         OPEN        CRO
                 MGLY        XYL         ISOP        NR

 1.700E+03   3.054E-03   1.885E-04   1.516E-09   1.995E-01   1.423E-06   3.457E-10   2.000E+04   3.358E-07   5.616E-05   1.553E-06
 1.370E+01   2.884E-02   7.317E-06   3.720E-05   2.671E-03   6.114E-01   6.556E-03   4.120E-03   9.795E-06   4.344E-05   5.704E-03
             9.550E-02   3.139E-05   9.619E-11   4.313E-05   7.738E-04   8.156E-04   4.435E-05   6.291E-09   1.396E-05   3.956E-08
             3.833E-05   5.754E-05   0.000E+00   2.980E-02

 NET RATES  -2.944E-06  -3.845E-07   2.776E-07   1.794E-04   3.246E-08  -2.041E-09  -3.258E-05  -1.033E-08  -1.632E-07  -2.269E-09
             1.678E-05  -6.501E-08  -1.469E-07   1.885E-05  -9.055E-06  -1.336E-06  -3.838E-06  -2.732E-07  -1.184E-07  -5.181E-06
            -5.645E-05  -8.100E-08   1.298E-10   1.486E-07  -2.544E-06  -1.797E-06  -3.612E-07  -2.298E-11  -1.034E-07  -1.844E-09
            -1.784E-07   6.991E-08   0.000E+00   4.446E-06

 THE REACTION RATES ARE
        1.34E-03    6.14E-03    1.08E-03    6.37E-08    1.03E-08    6.74E-10    3.30E-05    4.64E-03    1.66E-04    1.44E-04
        2.25E-05    7.06E-06    3.47E-05    2.12E-05    1.17E-05    2.74E-09    7.94E-06    5.90E-08    7.88E-06    5.31E-12
        1.84E-13    5.93E-07    6.34E-07    2.40E-08    8.03E-16    1.66E-05    2.00E-06    1.28E-04    3.33E-04    3.33E-04
        8.36E-08    1.23E-05    9.98E-06    1.11E-06    2.28E-06    6.61E-05    3.30E-05    7.79E-06    1.44E-05    2.57E-09
        8.68E-09    4.20E-09    3.27E-05    2.17E-08    6.06E-07    3.34E-05    2.70E-04    2.75E-04    3.55E-07    5.28E-06
        7.75E-06    3.86E-05    2.05E-05    9.18E-06    6.46E-09    3.94E-10    5.91E-07    1.74E-07    6.96E-10    1.32E-09
        3.03E-06    4.83E-07    2.46E-06    1.42E-08    1.57E-06    9.08E-07    2.05E-06    2.42E-06    1.39E-07    2.06E-07
        4.30E-08    6.95E-07    3.35E-07    4.08E-07    0.00E+00    0.00E+00    0.00E+00    0.00E+00    9.83E-05    5.92E-06
        3.51E-06    2.98E-02

 THE PHOTOLYTIC RATE CONSTANTS ARE
        4.388E-01   2.326E-02   8.329E-04   1.488E+01   8.667E-02   4.140E-04   1.189E-03   2.191E-03   1.470E-04
        9.986E-03   1.065E-02


 THE CURRENT MIXING HEIGHT IS      1701.34

 THE CURRENT TEMPERATURE IS         303.00

 THE CURRENT ZENITH ANGLE IS         52.16
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       TIME      NMOC        NMOC/        NOX        NO2         O3         NO2        PAR
      (LDT )    TOTAL         NOX        TOTAL     FRACTION  (INSTANT)  (INSTANT)  (INSTANT)

      1800.     .14529    41.37748      .00351      .95428     .20800     .00335     .09338

  TIME         NO2          NO           O           O3          NO3         O1D         H2O         OH          HO2         N2O5
 INTERVAL      HNO3         HNO2         PNA         H2O2        CO          FORM        ALD2        C2O3        XO2         PAN
               PAR          XO2N         ROR         OLE         ETH         TOL         CRES        TO2         OPEN        CRO
               MGLY         XYL          ISOP        NR

 1.800E+03   3.351E-03   1.605E-04   1.210E-09   2.080E-01   2.027E-06   1.365E-10   2.000E+04   1.971E-07   4.005E-05   2.422E-06
 1.092E+01   2.968E-02   4.861E-06   2.910E-05   3.489E-03   6.110E-01   6.577E-03   3.982E-03   8.155E-06   3.185E-05   5.279E-03
             9.338E-02   2.193E-05   5.522E-11   5.802E-05   6.753E-04   7.473E-04   2.337E-05   3.547E-09   8.899E-06   2.470E-08
             3.463E-05   7.155E-05   0.000E+00   3.010E-02

 NET RATES   5.787E-06  -4.786E-07  -1.335E-06   1.086E-04   5.779E-08   6.372E-08  -1.407E-05   5.472E-08  -4.458E-07   2.281E-08
             1.124E-05  -3.483E-08  -7.712E-08   8.571E-06  -3.761E-06   2.001E-06  -1.393E-06  -1.042E-07  -2.279E-07  -8.008E-06
            -2.403E-05  -1.707E-07  -7.656E-11   7.725E-08  -1.156E-06  -7.499E-07  -3.554E-07   8.829E-11  -6.883E-08  -3.482E-09
             1.184E-08   1.531E-07   0.000E+00   3.839E-06

 THE REACTION RATES ARE
      1.12E-03     4.90E-03     9.60E-04     5.57E-08     9.01E-09     4.58E-10     3.78E-05     3.70E-03     6.57E-05     5.67E-05
      8.90E-06     4.32E-06     2.58E-05     2.30E-05     1.42E-05     4.29E-09     1.24E-05     9.20E-08     1.23E-05     3.85E-12
      1.72E-13     2.97E-07     3.22E-07     9.36E-09     3.54E-16     1.07E-05     1.21E-06     7.78E-05     2.61E-04     2.61E-04
      3.84E-08     6.24E-06     5.07E-06     9.87E-07     1.75E-06     3.88E-05     1.94E-05     4.71E-06     9.84E-06     2.05E-09
      1.24E-08     3.24E-09     1.86E-05     2.99E-08     2.93E-07     2.36E-05     2.46E-04     2.54E-04     2.46E-07     3.13E-06
      4.55E-06     2.21E-05     1.18E-05     5.27E-06     4.07E-09     4.23E-10     4.67E-07     2.44E-07     1.33E-09     9.22E-10
      1.55E-06     4.39E-07     1.32E-06     6.83E-09     8.87E-07     2.81E-07     1.54E-06     1.66E-06     5.35E-08     7.72E-08
      2.85E-08     5.07E-07     1.77E-07     2.22E-07     0.00E+00     0.00E+00     0.00E+00     0.00E+00     6.14E-05     3.52E-06
      1.89E-06     3.01E-02

 THE PHOTOLYTIC RATE CONSTANTS ARE
        3.355E-01    1.778E-02    3.158E-04    1.137E+01    6.625E-02    2.828E-04    7.163E-04    1.496E-03    7.366E-05
        6.017E-03    6.418E-03


 THE CURRENT MIXING HEIGHT IS     1701.34

 THE CURRENT TEMPERATURE IS        303.00

 THE CURRENT ZENITH ANGLE IS        63.80
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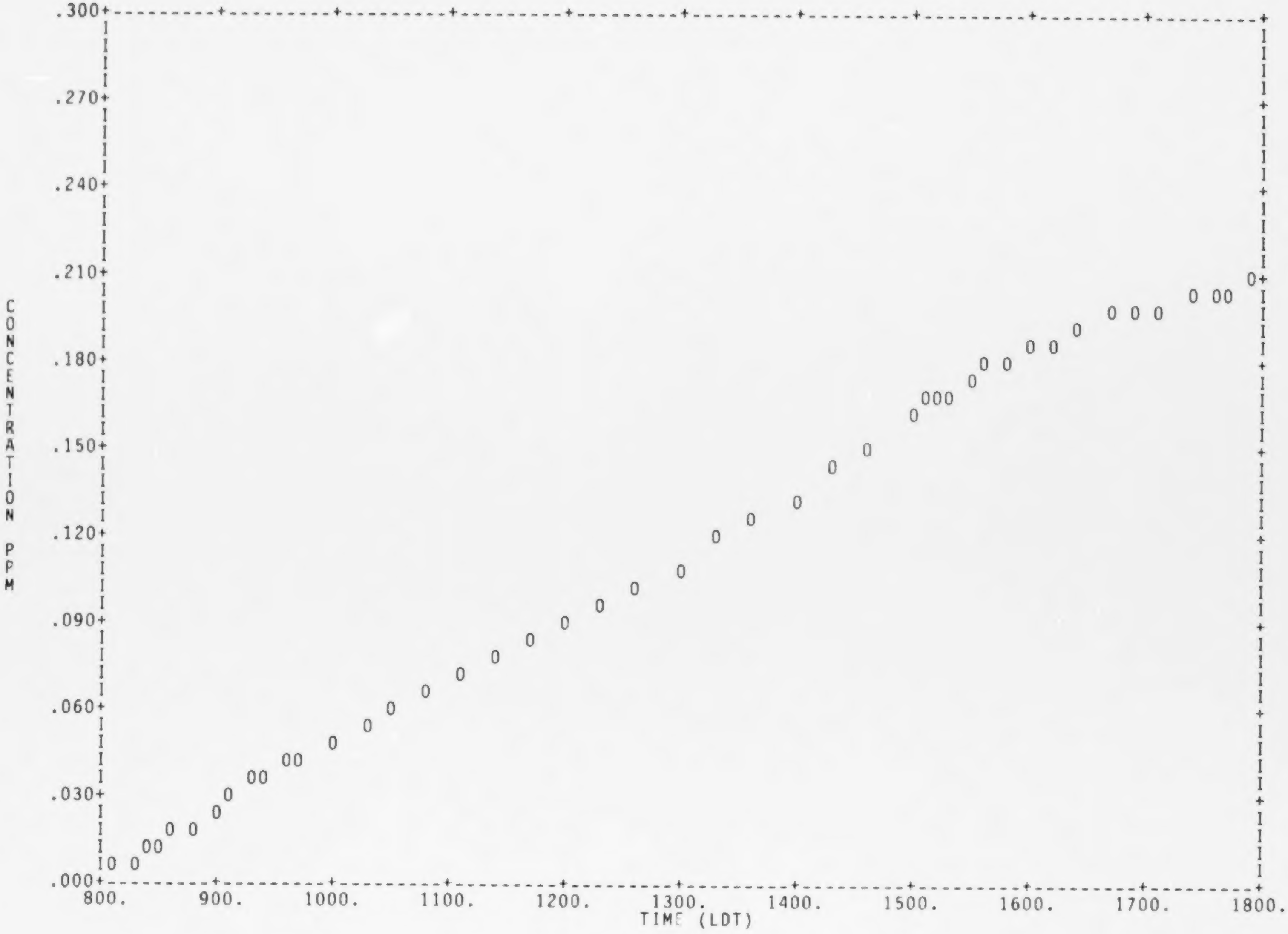
MAXIMUM O3    NOT REACHED, THE LAST ONE HOUR AVERAGE WAS  .20412 PPM.

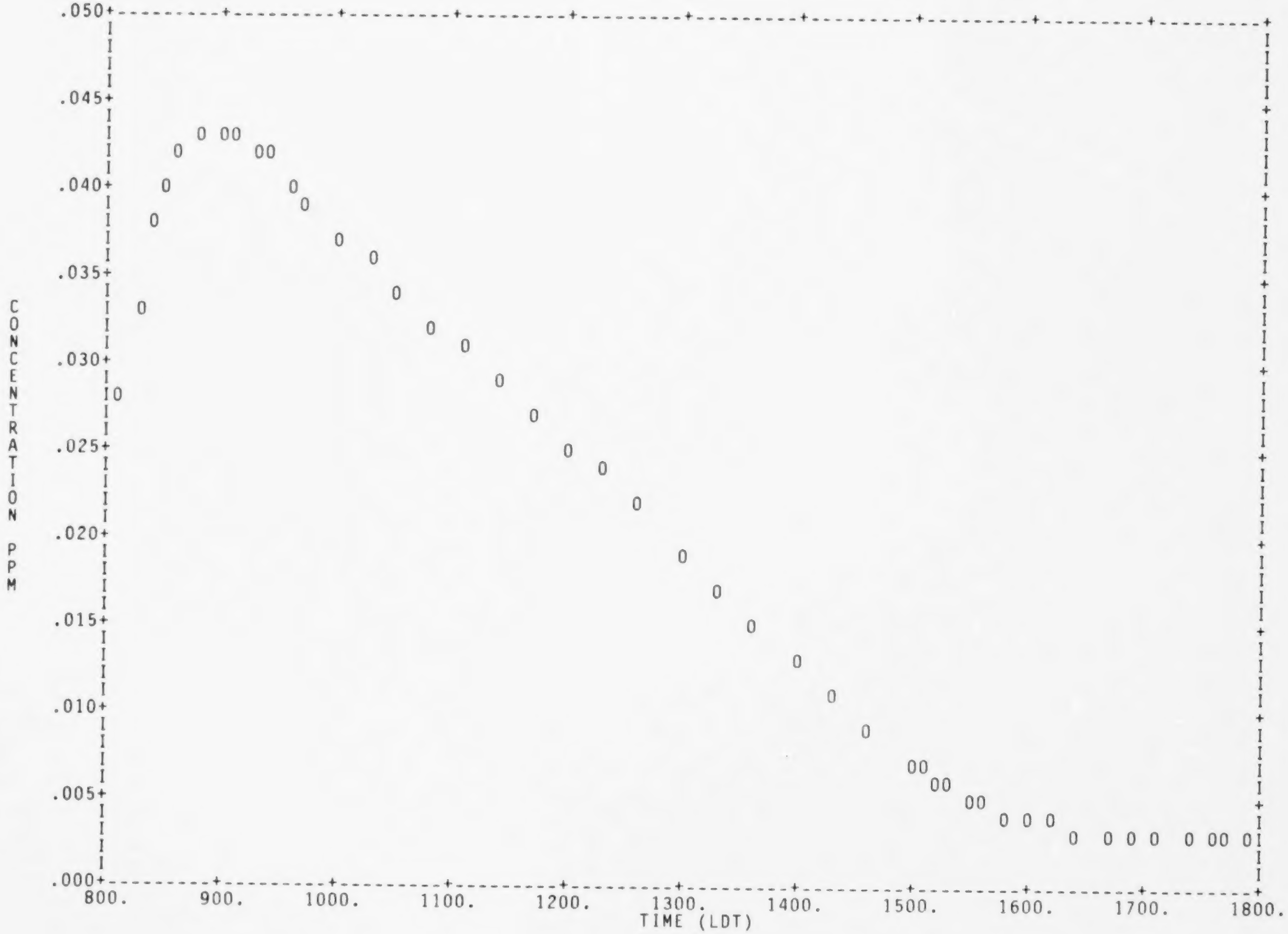
MAXIMUM ONE HOUR AVE NO2   =  .04243 CENTERED AT  904. LDT

MAXIMUM ONE HOUR AVE PAR   =  .42444 CENTERED AT  830. LDT
```



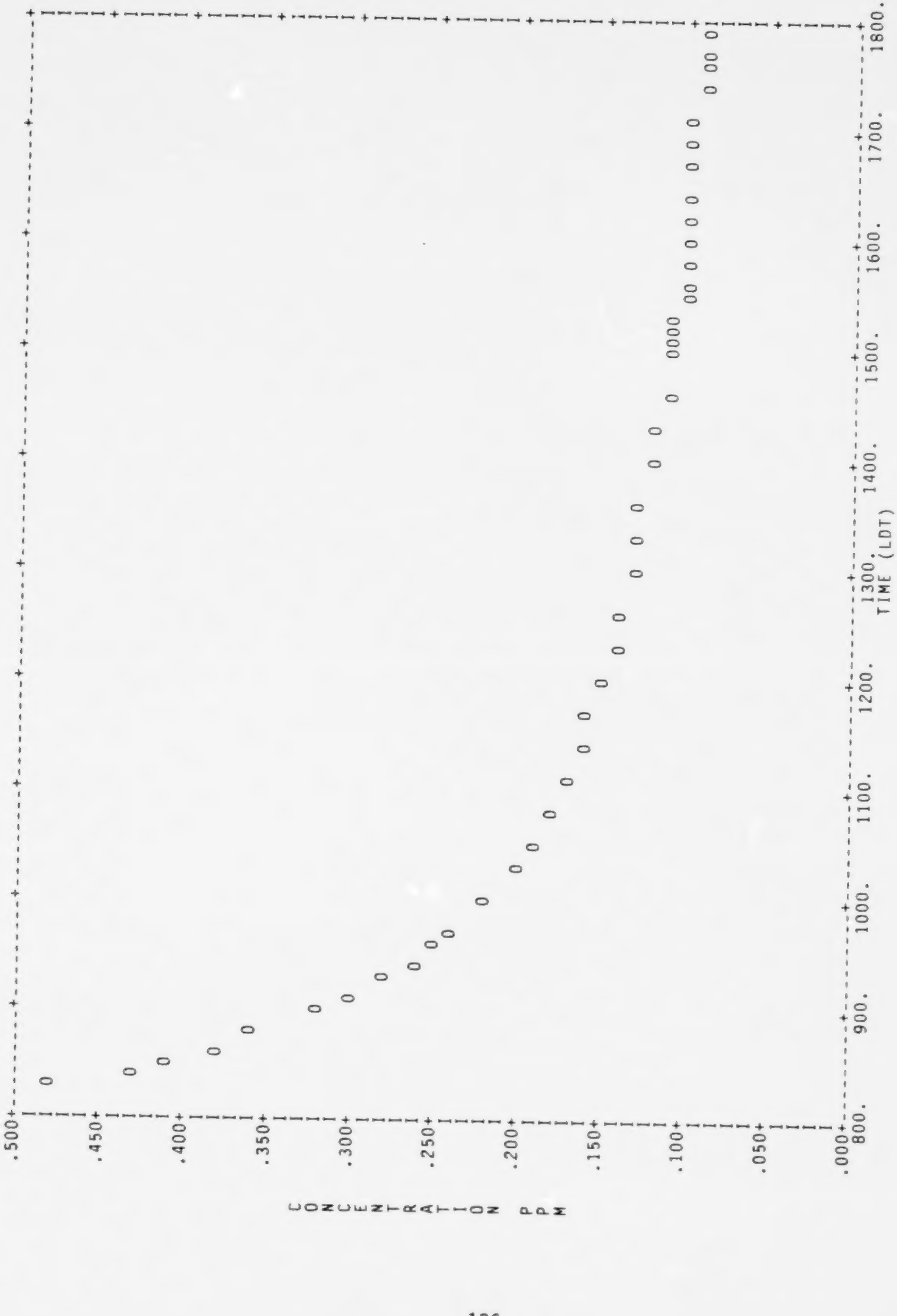
EXAMPLE 1 - SINGLE CALCULATION

03 CONCENTRATION AS A FUNCTION OF TIME



EXAMPLE 1 - SINGLE CALCULATION

NO2 CONCENTRATION AS A FUNCTION OF TIME



EXAMPLE 1 - SINGLE CALCULATION

PAR CONCENTRATION AS A FUNCTION OF TIME

EXHIBIT 3

```
(   1)          1         2         3         4         5         6         7
(   2) 123456789012345678901234567890123456789012345678901234567890123456789012
(   3)
(   4) MECH      82.       11.       10.
(   5) 1.        8.        9.        14.       23.       34.       38.
(   6) 39.       45.       69.       74.
(   7) ETH       OLE       ALD2      FORM      TOL       XYL       PAR
(   8) ISOP      MEOH      NR
(   9) 2.        2.        2.        1.        7.        8.        1.
(  10) 4.        1.        1.
(  11) NO2               1     NO          O                  1.
(  12) O                 2     O3                              4.323E+6  -1175.
(  13) O3    NO          3     NO2                            26.64       1370.
(  14) O     NO2         4     NO                             13750.
(  15) O     NO2         5     NO3                            2309.       -687.
(  16) O     NO          6     NO2                            2438.       -602.
(  17) NO2   O3          7     NO3                            0.04731     2450.
(  18) O3                8     O                              0.053
(  19) O3                9     O1D                            1.0
(  20) O1D              10     O                               4.246E+5   -390.
(  21) O1D   H2O        112.00 OH                             3.26
(  22) O3    OH         12     HO2                            100.         940.
(  23) O3    HO2        13     OH                             3.0          580.
(  24) NO3              140.89 NO2    0.89 O      0.11 NO     33.9
(  25) NO3   NO         15 2.  NO2                            44160.      -250.
(  26) NO3   NO2        16     NO          NO2                0.5901      1230.
(  27) NO3   NO2        17     N2O5                           1853.       -256.
(  28) N2O5  H2O        18 2.  HNO3                              1.9E-6
(  29) N2O5             19     NO3         NO2                2.776      10897.
(  30) NO    NO         20 2.  NO2                             1.539E-4   -530.
(  31) NO    NO2   H2O  21 2.  HNO2                             1.6E-11
(  32) NO    OH         22     HNO2                           9799.       -806.
(  33) HNO2             23     NO          OH                 0.1975
(  34) OH    HNO2       24     NO2                            9770.
(  35) HNO2  HNO2       25     NO          NO2                   1.5E-5
(  36) NO2   OH         26     HNO3                           16820.      -713.
(  37) OH    HNO3       27     NO3                            217.9      -1000.
(  38) HO2   NO         28     OH          NO2                12270.      -240.
(  39) HO2   NO2        29     PNA                            2025.       -749.
(  40) PNA              30     HO2         NO2                5.115      10121.
(  41) OH    PNA        31     NO2                            6833.       -380.
(  42) HO2   HO2        32     H2O2                           4144.      -1150.
(  43) HO2   HO2   H2O  33     H2O2                           0.2181     -5800.
(  44) H2O2             34 2.  OH                             0.189
(  45) OH    H2O2       35     HO2                            2520.        187.
(  46) OH    CO         36     HO2                            322.
(  47) FORM  OH         37     HO2         CO                 15000.
(  48) FORM             38 2.  HO2         CO                 1.00
(  49) FORM             39     CO                             1.00
(  50) FORM  O          40     OH          HO2         CO     237.        1550.
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EXHIBIT 3. Continued.

```
(   51) FORM  NO3         41      HNO3         HO2          CO      0.93
(   52) ALD2  O           42      C2O3         OH                   636.         986.
(   53) ALD2  OH          43      C2O3                              24000.      -250.
(   54) ALD2  NO3         44      C2O3         HNO3                 3.7
(   55) ALD2              45      FORM*   2.0  HO2          CO      1.0
(   56)       XO2
(   57) C2O3  NO          46      FORM*        NO2          HO2     18315.      -250.
(   58)       XO2
(   59) C2O3  NO2         47      PAN                               12230.     -5500.
(   60) PAN               48      C2O3         NO2                  0.0222     14000.
(   61) C2O3  C2O3        492.    FORM   2.0   XO2    2.0   HO2     3700.
(   62) C2O3  HO2         500.79  FORM*  0.79  XO2    0.79  HO2     9600.
(   63) 0.79  OH
(   64) OH                51      FORM         XO2          HO2     21.         1710.
(   65) PAR   OH          520.87  XO2 *  0.130 XO2N   0.11  HO2     1203.0
(   66) 0.11  ALD2  -0.11 PAR     0.76   ROR
(   67) ROR               530.96  XO2 *  1.1   ALD2   0.94  HO2     137100.     8000.
(   68) -2.1  PAR   0.04  XO2N    0.02   ROR
(   69) ROR               54      HO2                               95445.
(   70) ROR   NO2         55                                        22000.
(   71) O     OLE         560.63  ALD2*  0.38  HO2    0.28  XO2     5920.        324.
(   72) 0.30  CO    0.20  FORM    0.02   XO2N   0.22 PAR    0.2  OH
(   73) OH    OLE         57      FORM*        ALD2   -1.0  PAR     42000.      -504.
(   74)       XO2          HO2
(   75) O3    OLE         580.5   ALD2*  0.740 FORM   0.220 XO2     0.0180      2105.
(   76) 0.10  OH    0.330 CO      0.44   HO2   -1.0   PAR
(   77) NO3   OLE         590.91  XO2 *  1.0   FORM   0.09  XO2N    11.35
(   78) 1.0   ALD2  1.0   NO2     -1.0   PAR
(   79) O     ETH         60      FORM*  1.7   HO2          CO      1080.        792.
(   80) 0.7   XO2   0.3    OH
(   81) OH    ETH         61      XO2 *  1.56  FORM   0.22  ALD2    11920.      -411.
(   82)       HO2
(   83) O3    ETH         62      FORM   0.42  CO     0.12  HO2     0.002702    2633.
(   84) TOL   OH          630.44  HO2 *  0.08  XO2    0.36  CRES    9150.       -322.
(   85) 0.56  TO2
(   86) TO2   NO          640.90  NO2    0.90  HO2    0.90  OPEN    12000.
(   87) TO2               65      CRES         HO2                  250.
(   88) OH    CRES        660.40  CRO *  0.60  XO2    0.60  HO2     61000.
(   89) 0.30  OPEN
(   90) CRES  NO3         67      CRO          HNO3                 32500.
(   91) CRO   NO2         68                                        20000.
(   92) OPEN              69      C2O3         HO2          CO      8.40
(   93) OPEN  OH          70      XO2 *  2.    CO     2.    HO2     44000.
(   94)       C2O3         FORM
(   95) OPEN  O3          710.03  ALD2*  0.62  C2O3   0.70  FORM    0.015        500.
(   96) 0.03  XO2   0.69  CO      0.08   OH    0.76   HO2   0.20  MGLY
(   97) OH    XYL         720.70  HO2 *  0.50  XO2    0.20  CRES    36200.      -116.
(   98) 0.8   MGLY  1.1    PAR    0.30   TO2
(   99) OH    MGLY        73      XO2          C2O3                 26000.
(  100) MGLY              74      C2O3         HO2          CO      8.96
```

EXHIBIT 3. Continued.

```
(  101) O       ISOP          750.60 HO2 * 0.8    ALD2   0.55   OLE     27000.
(  102) 0.5     XO2    0.5    CO     0.450 ETH    0.9    PAR
(  103) OH      ISOP          76     XO2 *        FORM   0.67   HO2     142000.
(  104) 0.13    XO2N           ETH   0.4   MGLY    0.2   C2O3   0.2   ALD2
(  105) O3      ISOP          77     FORM* 0.4    ALD2   0.55   ETH     0.018
(  106) 0.20    MGLY   0.1     PAR   0.060 CO     0.44   HO2    0.1   OH
(  107) NO3     ISOP          78     XO2N                                470.
(  108) XO2     NO            79     NO2                                 12000.
(  109) XO2N    NO            80                                         1000.
(  110) XO2     XO2           81                                         2000.     -1300.
(  111) MEOH    OH            83     FORM         HO2                    1600.
(  112) NR                    82     NR                                     1.
(  113) ZENITH         7.
(  114) 9.             0.00461   0.00448   0.00413   0.00359   0.00287   0.00208
(  115) 0.00124        0.00054   0.00022   0.00013
(  116) 34.            0.00575   0.00573   0.00567   0.00554   0.00535   0.00508
(  117) 0.00463        0.00401   0.00347   0.00525
(  118) 38.            0.00370   0.00366   0.00356   0.00340   0.00314   0.00280
(  119) 0.00234        0.00174   0.00128   0.00177
(  120) 39.            0.00575   0.00573   0.00567   0.00554   0.00535   0.00508
(  121) 0.00463        0.00401   0.00347   0.00525
(  122) 45.          0.000589  0.000578  0.000550  0.000502  0.000435  0.000355
(  123) 0.000257     0.000158  0.000091  0.000094
(  124) 69.            0.00370   0.00366   0.00356   0.00340   0.00314   0.00280
(  125) 0.00234        0.00174   0.00128   0.00177
(  126) 74.            0.00370   0.00366   0.00356   0.00340   0.00314   0.00280
(  127) 0.00234        0.00174   0.00128   0.00177
(  128) TITL
(  129) EXAMPLE 2 - CB4 WITH METHANOL REACTION ADDED
(  130) PLAC       38.629    90.206    5.0       1986.     6.0       21.
(  131) TEST CITY
(  132) DILU       250.      1700.
(  133) TEMP       11.       293.      295.      297.      299.      301.
(  134) 303.       304.      306.      306.      305.      304.      302.
(  135) MOLE       -11.      2.        250.                .6        0.05
(  136) VOC        0.0005887 0.00048   0.0004712 0.0003256 0.0002018 0.00014
(  137) 0.0001362  0.0001093 0.0001075 0.0001312 0.00007
(  138) NOX        0.0001763 0.0001343 0.0001228 0.0000893 0.00006   0.0000413
(  139) 0.0000415  0.0000347 0.0000308 0.0000386 0.0000195
(  140) TRANS      .000      .080      0.        -10.      0.        0.009
(  141) 0.05       .034      .020      .037      .070      .042      .026
(  142) .497       0.        .01       .273
(  143) REAC       10.       .25
(  144) .0333      .0315     .0468     .0189     .0801     .1053     .5076
(  145) 0.         .1        .0756
(  146) DEPO       10.       3.
(  147) NO         .1        .1        .1        .1        .1        .1
(  148) .1         .1        .1        .1
(  149) NO2        2.5       2.5       2.5       2.5       2.5       2.5
(  150) 2.5        2.5       2.5       2.5
```

EXHIBIT 3. Concluded.

```
(  151) O3         1.886     1.886     1.886     1.886     1.886     1.886
(  152) 1.886      1.886     1.886     1.886
(  153) INIT       2.
(  154) H2O        CO
(  155) 15000.     .9
(  156) ALOFT      2.
(  157) PAN        CO
(  158) .0005      .2
(  159) SPEC       3.
(  160) O3         NO2       MEOH
(  161) CALC       1.        .1        1.
(  162)     BLANK
(  163)
(  164)          1         2         3         4         5         6         7
(  165) 123456789012345678901234567890123456789012345678901234567890123456789012
```

```
***************************************
*                                     *
*   OZONE ISOPLETH PLOTTING PACKAGE   *
*     WITH OPTIONAL MECHANISMS        *
*                                     *
*            O Z I P M                *
*                                     *
*           VERSION 4.00              *
*                                     *
*          DECEMBER, 1987             *
*                                     *
***************************************
```

EXHIBIT 4

```
THE INPUTS FOR THIS RUN ARE

     MECH      82.       11.       10.
     1.        8.        9.        14.
     39.       45.       69.       74.       23.       34.       38.
     ETH       OLE       ALD2      FORM      TOL       XYL       PAR
     ISOP      MEOH      NR
     2.        2.        2.        1.        7.        8.        1.
     4.        1.        1.
     NO2                    1       NO          O                          1.
     O                      2       O3                                       4.323E+6 -1175.
     O3     NO              3       NO2                                    26.64        1370.
     O      NO2             4       NO                                     13750.
     O      NO2             5       NO3                                    2309.        -687.
     O      NO              6       NO2                                    2438.        -602.
     NO2    O3              7       NO3                                    0.04731      2450.
     O3                     8       O                                      0.053
     O3                     9       O1D                                    1.0
     O1D                   10       O                                        4.246E+5   -390.
     O1D    H2O            112.00   OH                                     3.26
     O3     OH             12       HO2                                    100.          940.
     O3     HO2            13       OH                                     3.0           580.
     NO3                   140.89   NO2    0.89 O      0.11 NO             33.9
     NO3    NO             15 2.    NO2                                    44160.       -250.
     NO3    NO2            16       NO          NO2                        0.5901       1230.
     NO3    NO2            17       N2O5                                   1853.        -256.
     N2O5   H2O            18 2.    HNO3                                      1.9E-6
     N2O5                  19       NO3         NO2                        2.776       10897.
     NO     NO             20 2.    NO2                                      1.539E-4   -530.
     NO     NO2    H2O     21 2.    HNO2                                      1.6E-11
     NO     OH             22       HNO2                                   9799.        -806.
     HNO2                  23       NO          OH                         0.1975
     OH     HNO2           24       NO2                                    9770.
     HNO2   HNO2           25       NO          NO2                           1.5E-5
     NO2    OH             26       HNO3                                   16820.       -713.
     OH     HNO3           27       NO3                                    217.9       -1000.
     HO2    NO             28       OH          NO2                        12270.       -240.
     HO2    NO2            29       PNA                                    2025.        -749.
     PNA                   30       HO2         NO2                        5.115       10121.
     OH     PNA            31       NO2                                    6833.        -380.
     HO2    HO2            32       H2O2                                   4144.       -1150.
     HO2    HO2    H2O     33       H2O2                                   0.2181      -5800.
     H2O2                  34 2.    OH                                     0.189
     OH     H2O2           35       HO2                                    2520.         187.
     OH     CO             36       HO2                                    322.
     FORM   OH             37       HO2         CO                         15000.
     FORM                  38 2.    HO2         CO                         1.00
     FORM                  39       CO                                     1.00
     FORM   O              40       OH          HO2        CO              237.         1550.
     FORM   NO3            41       HNO3        HO2        CO              0.93
     ALD2   O              42       C2O3        OH                         636.          986.
```

```
THE INPUTS FOR THIS RUN ARE

ALD2  OH        43     C2O3                          24000.     -250.
ALD2  NO3       44     C2O3        HNO3              3.7
ALD2            45     FORM*   2.0 HO2         CO    1.0
      XO2
C2O3  NO        46     FORM*       NO2         HO2   18315.     -250.
      XO2
C2O3  NO2       47     PAN                           12230.    -5500.
PAN             48     C2O3        NO2               0.0222    14000.
C2O3  C2O3      492.   FORM   2.0  XO2     2.0 HO2   3700.
C2O3  HO2       500.79 FORM* 0.79  XO2   0.79  HO2   9600.
0.79  OH
OH              51     FORM        XO2         HO2   21.        1710.
PAR   OH        520.87 XO2 * 0.130 XO2N  0.11  HO2   1203.0
0.11  ALD2 -0.11 PAR   0.76  ROR
ROR             530.96 XO2 * 1.1   ALD2  0.94  HO2   137100.    8000.
-2.1  PAR   0.04 XO2N  0.02  ROR
ROR             54     HO2                           95445.
ROR   NO2       55                                   22000.
O     OLE       560.63 ALD2* 0.38  HO2   0.28  XO2   5920.       324.
0.30  CO    0.20 FORM  0.02  XO2N   0.22 PAR  0.2   OH
OH    OLE       57     FORM*       ALD2  -1.0  PAR   42000.     -504.
      XO2        HO2
O3    OLE       580.5  ALD2* 0.740 FORM  0.220 XO2   0.0180     2105.
0.10  OH   0.330 CO    0.44  HO2   -1.0  PAR
NO3   OLE       590.91 XO2 * 1.0   FORM  0.09  XO2N  11.35
1.0   ALD2  1.0  NO2   -1.0  PAR
O     ETH       60     FORM* 1.7   HO2         CO    1080.       792.
0.7   XO2   0.3  OH
OH    ETH       61     XO2 * 1.56  FORM  0.22  ALD2  11920.     -411.
      HO2
O3    ETH       62     FORM  0.42  CO    0.12  HO2   0.002702   2633.
TOL   OH        630.44 HO2 * 0.08  XO2   0.36  CRES  9150.      -322.
0.56  TO2
TO2   NO        640.90 NO2   0.90  HO2   0.90  OPEN  12000.
TO2             65     CRES        HO2               250.
OH    CRES      660.40 CRO * 0.60  XO2   0.60  HO2   61000.
0.30  OPEN
CRES  NO3       67     CRO         HNO3              32500.
CRO   NO2       68                                   20000.
OPEN            69     C2O3        HO2         CO    8.40
OPEN  OH        70     XO2 * 2.    CO    2.    HO2   44000.
      C2O3       FORM
OPEN  O3        710.03 ALD2* 0.62  C2O3  0.70  FORM  0.015       500.
0.03  XO2   0.69 CO    0.08  OH    0.76  HO2   0.20 MGLY
OH    XYL       720.70 HO2 * 0.50  XO2   0.20  CRES  36200.     -116.
0.8   MGLY  1.1  PAR   0.30  TO2
OH    MGLY      73     XO2         C2O3              26000.
MGLY            74     C2O3        HO2         CO    8.96
O     ISOP      750.60 HO2 * 0.8   ALD2  0.55  OLE   27000.
0.5   XO2   0.5  CO    0.450 ETH   0.9   PAR
```

THE INPUTS FOR THIS RUN ARE

```
OH     ISOP         76      XO2 *          FORM  0.67  HO2     142000.
0.13   XO2N          ETH    0.4    MGLY     0.2  C2O3  0.2    ALD2
O3     ISOP         77      FORM*  0.4     ALD2  0.55  ETH      0.018
0.20   MGLY   0.1    PAR    0.060  CO      0.44  HO2   0.1    OH
NO3    ISOP         78      XO2N                                470.
XO2    NO           79      NO2                                 12000.
XO2N   NO           80                                          1000.
XO2    XO2          81                                          2000.      -1300.
MEOH   OH           83      FORM           HO2                  1600.
NR                  82      NR                                     1.
ZENITH        7.
9.           0.00461    0.00448    0.00413    0.00359    0.00287    0.00208
0.00124      0.00054    0.00022    0.00013
34.          0.00575    0.00573    0.00567    0.00554    0.00535    0.00508
0.00463      0.00401    0.00347    0.00525
38.          0.00370    0.00366    0.00356    0.00340    0.00314    0.00280
0.00234      0.00174    0.00128    0.00177
39.          0.00575    0.00573    0.00567    0.00554    0.00535    0.00508
0.00463      0.00401    0.00347    0.00525
45.         0.000589   0.000578   0.000550   0.000502   0.000435   0.000355
0.000257    0.000158   0.000091   0.000094
69.          0.00370    0.00366    0.00356    0.00340    0.00314    0.00280
0.00234      0.00174    0.00128    0.00177
74.          0.00370    0.00366    0.00356    0.00340    0.00314    0.00280
0.00234      0.00174    0.00128    0.00177
TITL
EXAMPLE 2 - CB4 WITH METHANOL REACTION ADDED
PLAC        38.629     90.206     5.0        1986.      6.0        21.
TEST CITY
DILU        250.       1700.
TEMP        11.        293.       295.       297.       299.       301.
303.        304.       306.       306.       305.       304.       302.
MOLE        -11.       2.         250.                  .6         0.05
VOC         0.0005887  0.00048    0.0004712  0.0003256  0.0002018  0.00014
0.0001362   0.0001093  0.0001075  0.0001312  0.00007
NOX         0.0001763  0.0001343  0.0001228  0.0000893  0.00006    0.0000413
0.0000415   0.0000347  0.0000308  0.0000386  0.0000195
TRANS       .000       .080       0.         -10.       0.         0.009
0.05        .034       .020       .037       .070       .042       .026
.497        0.         .01        .273
REAC        10.        .25
.0333       .0315      .0468      .0189      .0801      .1053      .5076
0.          .1         .0756
DEPO        10.        3.
NO          .1         .1         .1         .1         .1         .1
.1          .1         .1         .1
NO2         2.5        2.5        2.5        2.5        2.5        2.5
2.5         2.5        2.5        2.5
O3          1.886      1.886      1.886      1.886      1.886      1.886
1.886       1.886      1.886      1.886
```

```
THE INPUTS FOR THIS RUN ARE

        INIT      2.
        H20       CO
        15000.    .9
        ALOFT     2.
        PAN       CO
        .0005     .2
        SPEC      3.
        03        N02       MEOH
        CALC      1.        .1        1.
            BLANK
```

```
THE REACTIONS                                                                                     RATE CONSTANT  ACT. ENERGY(K)
  1        NO2                          =      NO    +    O                                        1.000E+00      0.000E+00
  2        O                            =      O3                                                 4.323E+06     -1.175E+03
  3        O3    +    NO                =      NO2                                                2.664E+01      1.370E+03
  4        O     +    NO2               =      NO                                                 1.375E+04      0.000E+00
  5        O     +    NO2               =      NO3                                                2.309E+03     -6.870E+02
  6        O     +    NO                =      NO2                                                2.438E+03     -6.020E+02
  7        NO2   +    O3                =      NO3                                                4.731E-02      2.450E+03
  8        O3                           =      O                                                  5.300E-02      0.000E+00
  9        O3                           =      O1D                                                1.000E+00      0.000E+00
 10        O1D                          =      O                                                  4.246E+05     -3.900E+02
 11        O1D   +    H2O               =    2 OH                                                 3.260E+00      0.000E+00
 12        O3    +    OH                =      HO2                                                1.000E+02      9.400E+02
 13        O3    +    HO2               =      OH                                                 3.000E+00      5.800E+02
 14        NO3                          = 0.89 NO2   + 0.89 O    + 0.11 NO                        3.390E+01      0.000E+00
 15        NO3   +    NO                =    2 NO2                                                4.416E+04     -2.500E+02
 16        NO3   +    NO2               =      NO    +    NO2                                     5.901E-01      1.230E+03
 17        NO3   +    NO2               =      N2O5                                               1.853E+03     -2.560E+02
 18        N2O5  +    H2O               =    2 HNO3                                               1.900E-06      0.000E+00
 19        N2O5                         =      NO3   +    NO2                                     2.776E+00      1.090E+04
 20        NO    +    NO                =    2 NO2                                                1.539E-04     -5.300E+02
 21        NO    +    NO2   +    H2O    =    2 HNO2                                               1.600E-11      0.000E+00
 22        NO    +    OH                =      HNO2                                               9.799E+03     -8.060E+02
 23        HNO2                         =      NO    +    OH                                      1.975E-01      0.000E+00
 24        OH    +    HNO2              =      NO2                                                9.770E+03      0.000E+00
 25        HNO2  +    HNO2              =      NO    +    NO2                                     1.500E-05      0.000E+00
```

```
THE REACTIONS
                                                                                    RATE CONSTANT  ACT. ENERGY(K)
 26      NO2  +   OH                =     HNO3                                       1.682E+04     -7.130E+02
 27      OH   +   HNO3              =     NO3                                        2.179E+02     -1.000E+03
 28      HO2  +   NO                =     OH   +   NO2                                1.227E+04     -2.400E+02
 29      HO2  +   NO2               =     PNA                                        2.025E+03     -7.490E+02
 30      PNA                        =     HO2  +   NO2                                5.115E+00      1.012E+04
 31      OH   +   PNA               =     NO2                                        6.833E+03     -3.800E+02
 32      HO2  +   HO2               =     H2O2                                       4.144E+03     -1.150E+03
 33      HO2  +   HO2  +   H2O      =     H2O2                                       2.181E-01     -5.800E+03
 34      H2O2                       =   2 OH                                         1.890E-01      0.000E+00
 35      OH   +   H2O2              =     HO2                                        2.520E+03      1.870E+02
 36      OH   +   CO                =     HO2                                        3.220E+02      0.000E+00
 37      FORM +   OH                =     HO2  +   CO                                 1.500E+04      0.000E+00
 38      FORM                       =   2 HO2  +   CO                                 1.000E+00      0.000E+00
 39      FORM                       =     CO                                         1.000E+00      0.000E+00
 40      FORM +   O                 =     OH   +   HO2  +   CO                        2.370E+02      1.550E+03
 41      FORM +   NO3               =     HNO3 +   HO2  +   CO                        9.300E-01      0.000E+00
 42      ALD2 +   O                 =     C2O3 +   OH                                 6.360E+02      9.860E+02
 43      ALD2 +   OH                =     C2O3                                       2.400E+04     -2.500E+02
 44      ALD2 +   NO3               =     C2O3 +   HNO3                               3.700E+00      0.000E+00
 45      ALD2                       =     FORM +  2 HO2 +   CO   +   XO2              1.000E+00      0.000E+00

 46      C2O3 +   NO                =     FORM +   NO2  +   HO2  +   XO2              1.831E+04     -2.500E+02

 47      C2O3 +   NO2               =     PAN                                        1.223E+04     -5.500E+03
 48      PAN                        =     C2O3 +   NO2                                2.220E-02      1.400E+04
 49      C2O3 +   C2O3              =   2 FORM +  2 XO2 +  2 HO2                      3.700E+03      0.000E+00
 50      C2O3 +   HO2               = 0.79 FORM + 0.79 XO2 + 0.79 HO2 + 0.79 OH       9.600E+03      0.000E+00
```

```
THE REACTIONS                                                                                    RATE CONSTANT  ACT. ENERGY(K)
 51        OH                            =       FORM  +      XO2   +     HO2                     2.100E+01      1.710E+03
 52        PAR   +     OH                =   0.87 XO2  + 0.13 XO2N  + 0.11 HO2   + 0.11 ALD2     1.203E+03      0.000E+00
                                           - 0.11 PAR  + 0.76 ROR
 53        ROR                           =   0.96 XO2  +  1.1 ALD2  + 0.94 HO2   -  2.1 PAR      1.371E+05      8.000E+03
                                           + 0.04 XO2N + 0.02 ROR
 54        ROR                           =       HO2                                             9.545E+04      0.000E+00
 55        ROR   +     NO2               =                                                       2.200E+04      0.000E+00
 56        O     +     OLE               =   0.63 ALD2 + 0.38 HO2   + 0.28 XO2   +  0.3 CO       5.920E+03      3.240E+02
                                           +  0.2 FORM + 0.02 XO2N  + 0.22 PAR   +  0.2 OH
 57        OH    +     OLE               =       FORM  +      ALD2  -      PAR   +      XO2      4.200E+04     -5.040E+02
                                           +     HO2
 58        O3    +     OLE               =    0.5 ALD2 + 0.74 FORM  + 0.22 XO2   +  0.1 OH       1.800E-02      2.105E+03
                                           + 0.33 CO   + 0.44 HO2   -      PAR
 59        NO3   +     OLE               =   0.91 XO2  +      FORM  + 0.09 XO2N  +      ALD2     1.135E+01      0.000E+00
                                           +     NO2   -      PAR
 60        O     +     ETH               =       FORM  +  1.7 HO2   +      CO    +  0.7 XO2      1.080E+03      7.920E+02
                                           +  0.3 OH
 61        OH    +     ETH               =       XO2   + 1.56 FORM  + 0.22 ALD2  +      HO2      1.192E+04     -4.110E+02
 62        O3    +     ETH               =       FORM  + 0.42 CO    + 0.12 HO2                   2.702E-03      2.633E+03
 63        TOL   +     OH                =   0.44 HO2  + 0.08 XO2   + 0.36 CRES  + 0.56 TO2      9.150E+03     -3.220E+02
 64        TO2   +     NO                =    0.9 NO2  +  0.9 HO2   +  0.9 OPEN                  1.200E+04      0.000E+00
 65        TO2                           =       CRES  +      HO2                                2.500E+02      0.000E+00
 66        OH    +     CRES              =    0.4 CRO  +  0.6 XO2   +  0.6 HO2   +  0.3 OPEN     6.100E+04      0.000E+00
 67        CRES  +     NO3               =       CRO   +      HNO3                               3.250E+04      0.000E+00
 68        CRO   +     NO2               =                                                       2.000E+04      0.000E+00
 69        OPEN                          =       C2O3  +      HO2   +      CO                    8.400E+00      0.000E+00
 70        OPEN  +     OH                =       XO2   +    2 CO    +    2 HO2   +      C2O3     4.400E+04      0.000E+00
                                           +     FORM
```

```
THE REACTIONS
                                                                                                    RATE CONSTANT  ACT. ENERGY(K)
 71        OPEN  +      O3                =   0.03 ALD2   + 0.62 C2O3   +  0.7 FORM  + 0.03 XO2
                                            + 0.69 CO     + 0.08 OH     + 0.76 HO2   +  0.2 MGLY     1.500E-02      5.000E+02

 72        OH    +      XYL               =    0.7 HO2    +  0.5 XO2    +  0.2 CRES  +  0.8 MGLY     3.620E+04     -1.160E+02
                                            +  1.1 PAR    +  0.3 TO2

 73        OH    +      MGLY              =        XO2    +      C2O3                                2.600E+04      0.000E+00
 74        MGLY                           =        C2O3   +      HO2    +      CO                     8.960E+00      0.000E+00
 75        O     +      ISOP              =    0.6 HO2    +  0.8 ALD2   + 0.55 OLE   +  0.5 XO2      2.700E+04      0.000E+00
                                            +  0.5 CO     + 0.45 ETH    +  0.9 PAR

 76        OH    +      ISOP              =        XO2    +      FORM   + 0.67 HO2   + 0.13 XO2N     1.420E+05      0.000E+00
                                            +      ETH    +  0.4 MGLY   +  0.2 C2O3  +  0.2 ALD2

 77        O3    +      ISOP              =        FORM   +  0.4 ALD2   + 0.55 ETH   +  0.2 MGLY     1.800E-02      0.000E+00
                                            +  0.1 PAR    + 0.06 CO     + 0.44 HO2   +  0.1 OH

 78        NO3   +      ISOP              =        XO2N                                               4.700E+02      0.000E+00
 79        XO2   +      NO                =        NO2                                                1.200E+04      0.000E+00
 80        XO2N  +      NO                =                                                           1.000E+03      0.000E+00
 81        XO2   +      XO2               =                                                           2.000E+03     -1.300E+03
 83        MEOH  +      OH                =        FORM   +      HO2                                  1.600E+03      0.000E+00
 82        NR                             =        NR                                                 1.000E+00      0.000E+00
```

THE FOLLOWING PHOTOLYSIS RATE CONSTANTS ARE USED

REACTION NO.	SPECIES	ZENITH ANGLE (DEG)									
		0	10	20	30	40	50	60	70	78	86
1	NO2	5.89E-01	5.85E-01	5.71E-01	5.47E-01	5.09E-01	4.54E-01	3.74E-01	2.58E-01	1.34E-01	2.42E-02
8	O3	3.12E-02	3.10E-02	3.03E-02	2.90E-02	2.70E-02	2.40E-02	1.98E-02	1.37E-02	7.11E-03	1.28E-03
9	O3	2.72E-03	2.62E-03	2.36E-03	1.96E-03	1.46E-03	9.44E-04	4.64E-04	1.39E-04	2.95E-05	3.15E-06
14	NO3	2.00E+01	1.98E+01	1.94E+01	1.85E+01	1.73E+01	1.54E+01	1.27E+01	8.74E+00	4.55E+00	8.20E-01
23	HNO2	1.16E-01	1.16E-01	1.13E-01	1.08E-01	1.01E-01	8.96E-02	7.39E-02	5.09E-02	2.65E-02	4.78E-03
34	H2O2	6.40E-04	6.34E-04	6.12E-04	5.73E-04	5.15E-04	4.36E-04	3.27E-04	1.95E-04	8.79E-05	2.40E-05
38	FORM	2.18E-03	2.14E-03	2.03E-03	1.86E-03	1.60E-03	1.27E-03	8.75E-04	4.49E-04	1.72E-04	4.28E-05
39	FORM	3.39E-03	3.35E-03	3.24E-03	3.03E-03	2.72E-03	2.30E-03	1.73E-03	1.03E-03	4.65E-04	1.27E-04
45	ALD2	3.47E-04	3.38E-04	3.14E-04	2.75E-04	2.22E-04	1.61E-04	9.61E-05	4.07E-05	1.22E-05	2.27E-06
69	OPEN	1.83E-02	1.80E-02	1.71E-02	1.56E-02	1.34E-02	1.07E-02	7.35E-03	3.77E-03	1.44E-03	3.60E-04
74	MGLY	1.95E-02	1.92E-02	1.82E-02	1.67E-02	1.43E-02	1.14E-02	7.84E-03	4.02E-03	1.54E-03	3.84E-04

```
EXAMPLE 2 - CB4 WITH METHANOL REACTION ADDED


PHOTOLYTIC RATE CONSTANTS CALCULATED FOR

         TEST CITY

LATITUDE      38.629
LONGITUDE     90.206
TIME ZONE     5.0
DATE          6      21    1986
TIME          800    TO    1800      LOCAL DAYLIGHT TIME


DILUTION DETERMINED FROM THE FOLLOWING
INVERSION HEIGHTS      INITIAL    250.      FINAL       1700.
TIMING                 START      800.      STOP        1500.


MIXING HEIGHTS (AT THE BEGINNING OF EACH HOUR)
TIME        800      900     1000     1100     1200     1300     1400     1500

HEIGHT     250.0    503.1    821.2   1119.5   1340.2   1496.2   1610.8   1700.0


TEMPERATURE (AT THE BEGINNING OF EACH HOUR)
HOUR          0        1        2        3        4        5        6        7        8        9
             10       11

TEMP       293.0    295.0    297.0    299.0    301.0    303.0    304.0    306.0    306.0    305.0
           304.0    302.0

REACTIVITY

EMISSIONS        ETH  FRACTION  .033   OLE  FRACTION  .032   ALD2 FRACTION  .047

EMISSIONS        FORM FRACTION  .019   TOL  FRACTION  .080   XYL  FRACTION  .105

EMISSIONS        PAR  FRACTION  .508   ISOP FRACTION  .000   MEOH FRACTION  .100
EMISSIONS        NR   FRACTION  .076

ALOFT            ETH  FRACTION  .034   OLE  FRACTION  .020   ALD2 FRACTION  .037

ALOFT            FORM FRACTION  .070   TOL  FRACTION  .042   XYL  FRACTION  .026

ALOFT            PAR  FRACTION  .497   ISOP FRACTION  .000   MEOH FRACTION  .010

ALOFT            NR   FRACTION  .273

NO2/NOX         .250
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```
TRANSPORTED CONCENTRATIONS

SURFACE LAYER        H2O  15000.000     CO           .900
ALOFT                OZONE     .080     HYDROCARBON  .050    NOX      .009 PPM

ALOFT                PAN       .001     CO           .200


CONTINUOUS EMISSIONS (EXPRESSED AS FRACTION OF THE INITIAL PRECURSORS)
SPECIES      HOUR          1     2     3     4     5     6     7     8     9    10
                          11

  VOC      FRACTION      .096  .078  .077  .053  .033  .023  .022  .018  .018  .021
                         .011

  NOX      FRACTION      .345  .263  .240  .175  .117  .081  .081  .068  .060  .076
                         .038


SURFACE DEPOSITION RATES (CM/SEC)

SPECIES      HOUR          1     2     3     4     5     6     7     8     9    10

  NO       RATE          .100  .100  .100  .100  .100  .100  .100  .100  .100  .100

  NO2      RATE         2.500 2.500 2.500 2.500 2.500 2.500 2.500 2.500 2.500 2.500

  O3       RATE         1.886 1.886 1.886 1.886 1.886 1.886 1.886 1.886 1.886 1.886
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                         EXAMPLE 2 - CB4 WITH METHANOL REACTION ADDED

INITIAL CONCENTRATIONS
            H2O        CO
         1.500E+04  9.000E-01

THE ERROR TOLERANCE IS  3.000E-03

THE TEMPERATURE USED IS  2.930E+02

THE MIXING HEIGHT IS  2.50E+02

THE RATE CONSTANTS USED WERE


   3.248E-01   4.624E+06   2.463E+01   1.375E+04   2.402E+03   2.524E+03   4.112E-02   1.722E-02   2.845E-04   4.342E+05

   3.260E+00   9.476E+01   2.902E+00   1.101E+01   4.480E+04   5.500E-01   1.880E+03   1.900E-06   1.487E+00   1.586E-04

   1.600E-11   1.026E+04   6.416E-02   9.770E+03   1.500E-05   1.752E+04   2.307E+02   1.244E+04   2.114E+03   2.865E+00

   6.983E+03   4.426E+03   3.040E-01   2.708E-04   2.493E+03   3.220E+02   1.500E+04   6.778E-04   1.433E-03   2.169E+02

   9.300E-01   6.011E+02   2.435E+04   3.700E+00   6.830E-05   1.858E+04   1.676E+04   9.958E-03   3.700E+03   9.600E+03

   1.904E+01   1.203E+03   8.671E+04   9.545E+04   2.200E+04   5.811E+03   4.323E+04   1.596E-02   1.135E+01   1.032E+03

   1.220E+04   2.324E-03   9.320E+03   1.200E+04   2.500E+02   6.100E+04   3.250E+04   2.000E+04   5.694E-03   4.400E+04

   1.458E-02   3.644E+04   2.600E+04   6.074E-03   2.700E+04   1.420E+05   1.800E-02   4.700E+02   1.200E+04   1.000E+03

   2.155E+03   1.000E+00   1.600E+03

THE PHOTOLYSIS REACTIONS ARE

          1           8           9          14          23          34          38          39          45

         69          74

THE PHOTOLYTIC RATE CONSTANTS ARE
        3.248E-01   1.722E-02   2.845E-04   1.101E+01   6.416E-02   2.708E-04   6.778E-04   1.433E-03   6.830E-05
        5.694E-03   6.074E-03
```

```
          TIME      NMOC       NMOC/        NOX          NO2         O3          NO2          MEOH
         (LDT )     TOTAL       NOX         TOTAL      FRACTION   (INSTANT)   (INSTANT)   (INSTANT)

          800.      .99910     9.99100      .10000       .25000      .00000       .02500       .10000

  TIME          NO2         NO          O           O3          NO3         O1D         H2O         OH          HO2         N2O5
INTERVAL        HNO3        HNO2        PNA         H2O2        CO          FORM        ALD2        C2O3        XO2         PAN
                PAR         XO2N        ROR         OLE         ETH         TOL         CRES        TO2         OPEN        CRO
                MGLY        XYL         ISOP        NR          MEOH

 8.000E+02   2.500E-02   7.500E-02   0.000E+00   0.000E+00   0.000E+00   0.000E+00   1.500E+04   0.000E+00   0.000E+00   0.000E+00
 1.000E-10   0.000E+00   0.000E+00   0.000E+00   0.000E+00   9.000E-01   1.890E-02   2.340E-02   0.000E+00   0.000E+00   0.000E+00
             5.076E-01   0.000E+00   0.000E+00   1.575E-02   1.665E-02   1.144E-02   0.000E+00   0.000E+00   0.000E+00   0.000E+00
             0.000E+00   1.316E-02   0.000E+00   7.560E-02   1.000E-01

NET RATES   -8.446E-03   7.685E-03   8.121E-03   1.027E-03   0.000E+00   0.000E+00  -4.500E-10   0.000E+00   2.882E-05   0.000E+00
             0.000E+00   9.000E-10   0.000E+00   0.000E+00  -8.942E-03  -2.057E-04  -2.526E-04   0.000E+00   1.598E-06   6.417E-06
            -5.384E-03   0.000E+00   0.000E+00  -1.705E-04  -1.761E-04  -1.247E-04   0.000E+00   0.000E+00   0.000E+00   0.000E+00
             0.000E+00  -1.458E-04   0.000E+00  -6.741E-04  -1.117E-03

THE REACTION RATES ARE
     8.12E-03     0.00E+00     0.00E+00     0.00E+00     0.00E+00     0.00E+00     0.00E+00     0.00E+00     0.00E+00     0.00E+00
     0.00E+00     0.00E+00     0.00E+00     0.00E+00     0.00E+00     0.00E+00     0.00E+00     0.00E+00     0.00E+00     8.92E-07
     4.50E-10     0.00E+00     0.00E+00     0.00E+00     0.00E+00     0.00E+00     0.00E+00     0.00E+00     0.00E+00     0.00E+00
     0.00E+00     0.00E+00     0.00E+00     0.00E+00     0.00E+00     0.00E+00     0.00E+00     0.00E+00     0.00E+00     0.00E+00
     0.00E+00     0.00E+00     0.00E+00     0.00E+00     0.00E+00     0.00E+00     0.00E+00     1.28E-05     2.71E-05     0.00E+00
     0.00E+00     0.00E+00     0.00E+00     0.00E+00     1.60E-06     0.00E+00     0.00E+00     0.00E+00     0.00E+00     0.00E+00
     0.00E+00     0.00E+00     0.00E+00     0.00E+00     0.00E+00     0.00E+00     0.00E+00     0.00E+00     0.00E+00     0.00E+00
     0.00E+00     0.00E+00     0.00E+00     0.00E+00     0.00E+00     0.00E+00     0.00E+00     0.00E+00     0.00E+00     0.00E+00
     0.00E+00     7.56E-02     0.00E+00                                           0.00E+00     0.00E+00     0.00E+00     0.00E+00

THE PHOTOLYTIC RATE CONSTANTS ARE
        3.248E-01    1.722E-02    2.845E-04    1.101E+01    6.416E-02    2.708E-04    6.778E-04    1.433E-03    6.830E-05
        5.694E-03    6.074E-03


THE CURRENT MIXING HEIGHT IS        250.00

THE CURRENT TEMPERATURE IS          293.00

THE CURRENT ZENITH ANGLE IS          64.75
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     TIME      NMOC        NMOC/        NOX          NO2        O3          NO2         MEOH
    (LDT )     TOTAL       NOX          TOTAL        FRACTION   (INSTANT)   (INSTANT)   (INSTANT)

    900.       .56002      8.81899      .06350       .56931     .02260      .03615      .05446

 TIME           NO2         NO          O           O3          NO3         O1D         H2O         OH          HO2         N2O5
 INTERVAL       HNO3        HNO2        PNA         H2O2        CO          FORM        ALD2        C2O3        XO2         PAN
                PAR         XO2N        ROR         OLE         ETH         TOL         CRES        TO2         OPEN        CRO
                MGLY        XYL         ISOP        NR          MEOH

 9.000E+02   3.615E-02   2.735E-02   3.587E-09   2.260E-02   2.889E-08   3.701E-11   1.500E+04   5.645E-08   4.137E-07   9.866E-07
 9.637E+00   1.124E-03   1.806E-04   8.531E-06   2.861E-08   5.494E-01   1.221E-02   1.374E-02   3.094E-08   2.362E-07   5.381E-04
             2.869E-01   1.041E-07   7.458E-11   7.870E-03   9.204E-03   6.239E-03   2.359E-04   1.023E-08   1.217E-04   7.559E-10
             3.743E-04   6.642E-03   0.000E+00   4.802E-02   5.446E-02

 NET RATES  -5.312E-04   6.916E-05  -4.453E-04   1.305E-03  -2.610E-06  -1.438E-07  -1.839E-06  -5.107E-07  -8.730E-06   4.583E-07
             2.486E-05  -1.451E-06   7.085E-06   1.239E-09  -3.420E-03  -6.775E-05  -9.993E-05  -4.272E-06  -9.556E-07   1.301E-05
            -2.280E-03  -5.172E-08   1.293E-06  -8.410E-05  -7.788E-05  -5.405E-05   3.094E-06   2.460E-08   5.359E-07  -3.263E-11
             2.809E-06  -6.856E-05   0.000E+00  -2.870E-04  -4.690E-04

 THE REACTION RATES ARE
        1.56E-02     1.66E-02     1.52E-02     1.78E-06     3.11E-07     2.48E-07     3.36E-05     5.17E-04     1.77E-05     1.61E-05
        1.81E-06     1.21E-07     2.71E-08     4.23E-07     3.54E-05     5.74E-10     1.96E-06     2.81E-08     1.47E-06     1.19E-07
        2.37E-10     1.58E-05     1.54E-05     9.96E-08     4.89E-13     3.58E-05     1.46E-08     1.41E-04     3.16E-05     2.44E-05
        3.36E-09     7.58E-10     7.81E-10     1.16E-11     4.03E-12     9.99E-06     1.03E-05     1.41E-05     2.61E-05     9.50E-09
        3.28E-10     2.96E-08     1.89E-05     1.47E-09     1.93E-06     1.57E-05     1.87E-05     5.36E-06     3.54E-12     1.23E-10
        1.07E-06     1.95E-05     6.47E-06     7.12E-06     5.93E-08     1.64E-07     1.92E-05     2.84E-06     2.58E-09     3.41E-08
        6.34E-06     4.83E-07     3.28E-06     3.36E-06     2.56E-06     8.12E-07     2.21E-07     5.47E-07     1.18E-06     3.02E-07
        4.01E-08     1.37E-05     5.49E-07     3.86E-06     0.00E+00     0.00E+00     0.00E+00     0.00E+00     7.75E-05     2.85E-06
        1.20E-10     4.80E-02     4.92E-06

 THE PHOTOLYTIC RATE CONSTANTS ARE
          4.318E-01   2.288E-02    7.845E-04    1.464E+01    8.527E-02    4.039E-04    1.152E-03    2.137E-03    1.406E-04
          9.677E-03   1.032E-02


 THE CURRENT MIXING HEIGHT IS       503.11

 THE CURRENT TEMPERATURE IS         293.00

 THE CURRENT ZENITH ANGLE IS         53.12
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   TIME      NMOC        NMOC/        NOX         NO2         O3          NO2         MEOH
  (LDT )     TOTAL        NOX         TOTAL      FRACTION   (INSTANT)   (INSTANT)   (INSTANT)

  1000.      .37612     8.59213      .04378      .69311      .04279      .03034      .03568

  TIME          NO2          NO           O           O3           NO3          O1D          H2O          OH           HO2          N2O5
INTERVAL        HNO3         HNO2         PNA         H2O2         CO           FORM         ALD2         C2O3         XO2          PAN
                PAR          XO2N         ROR         OLE          ETH          TOL          CRES         TO2          OPEN         CRO
                MGLY         XYL          ISOP        NR           MEOH

1.000E+03    3.034E-02    1.343E-02    3.753E-09    4.279E-02    9.609E-08    1.249E-10    1.500E+04    9.284E-08    9.474E-07    2.172E-06
1.336E+01    2.750E-03    1.192E-04    1.283E-05    1.995E-07    4.164E-01    9.544E-03    9.829E-03    7.948E-08    5.321E-07    1.040E-03
             1.951E-01    2.389E-07    7.567E-11    4.367E-03    6.022E-03    4.049E-03    3.727E-04    1.407E-08    1.198E-04    3.310E-09
             4.402E-04    3.815E-03    0.000E+00    3.649E-02    3.568E-02

NET RATES   -1.010E-04   -1.222E-04    3.713E-07    2.822E-04   -5.252E-10   -1.906E-09   -6.170E-06   -2.484E-09    7.230E-09    1.133E-08
             3.101E-05   -3.834E-07    5.933E-08    5.451E-09   -1.362E-03   -2.558E-05   -3.999E-05    1.892E-10    7.968E-09    8.147E-06
            -9.644E-04    3.052E-09   -2.263E-10   -3.961E-05   -3.468E-05   -2.348E-05    1.614E-06    6.457E-11   -2.402E-07   -2.478E-11
             2.067E-07   -3.155E-05    0.000E+00   -1.197E-04   -1.961E-04

THE REACTION RATES ARE
      1.52E-02     1.64E-02     1.51E-02     1.57E-06     2.65E-07     1.24E-07     5.97E-05     1.14E-03     5.94E-05     5.32E-05
      6.11E-06     3.93E-07     1.21E-07     1.64E-06     5.72E-05     1.70E-09     5.42E-06     6.19E-08     5.33E-06     2.79E-08
      9.78E-11     1.23E-05     1.18E-05     1.08E-07     2.13E-13     4.78E-05     5.63E-08     1.57E-04     5.87E-05     5.86E-05
      8.18E-09     3.77E-09     3.14E-09     1.01E-10     4.66E-11     1.24E-05     1.33E-05     1.49E-05     2.55E-05     8.34E-09
      8.53E-10     2.32E-08     2.20E-05     3.49E-09     2.10E-06     1.96E-05     3.14E-05     1.97E-05     2.34E-11     7.23E-10
      1.91E-06     2.18E-05     9.48E-06     7.22E-06     5.05E-08     9.67E-08     1.71E-05     3.28E-06     4.76E-09     2.42E-08
      6.70E-06     6.76E-07     3.45E-06     2.27E-06     3.52E-06     2.11E-06     1.16E-06     2.01E-06     1.57E-06     4.89E-07
      7.64E-08     1.28E-05     1.06E-06     6.14E-06     0.00E+00     0.00E+00     0.00E+00     0.00E+00     8.58E-05     3.21E-06
      5.75E-10     3.65E-02     5.30E-06

THE PHOTOLYTIC RATE CONSTANTS ARE
        5.025E-01     2.663E-02     1.387E-03     1.704E+01     9.925E-02     5.053E-04     1.556E-03     2.673E-03     2.133E-04
        1.307E-02     1.394E-02


THE CURRENT MIXING HEIGHT IS      821.23

THE CURRENT TEMPERATURE IS        297.00

THE CURRENT ZENITH ANGLE IS        41.43
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    TIME       NMOC        NMOC/        NOX         NO2          O3          NO2          MEOH
   (LDT )      TOTAL        NOX        TOTAL      FRACTION    (INSTANT)    (INSTANT)    (INSTANT)

   1100.      .29472      8.76848     .03361      .74528      .05791       .02505       .02771

  TIME         NO2          NO           O           O3          NO3          O1D          H2O          OH           HO2          N2O5
INTERVAL       HNO3         HNO2         PNA         H2O2        CO           FORM         ALD2         C2O3         XO2          PAN
               PAR          XO2N         ROR         OLE         ETH          TOL          CRES         TO2          OPEN         CRO
               MGLY         XYL          ISOP        NR          MEOH

 1.100E+03   2.505E-02    8.562E-03    3.628E-09    5.791E-02    1.731E-07    2.406E-10    1.500E+04    1.485E-07    1.819E-06    2.529E-06
 1.858E+01   4.994E-03    1.094E-04    1.595E-05    8.674E-07    3.617E-01    8.700E-03    8.226E-03    1.809E-07    1.037E-06    1.531E-03
             1.555E-01    4.825E-07    8.687E-11    2.579E-03    4.509E-03    3.049E-03    4.328E-04    1.750E-08    1.082E-04    7.987E-09
             4.344E-04    2.396E-03    0.000E+00    3.170E-02    2.771E-02

 NET RATES  -6.341E-05   -7.564E-05   -7.705E-07    2.235E-04   -7.018E-08    4.347E-09   -1.185E-05    1.735E-07   -6.528E-08   -4.760E-09
             4.510E-05   -4.833E-08   -1.390E-08    1.948E-08   -5.699E-04   -5.347E-06   -1.780E-05   -1.462E-08   -6.072E-08    8.341E-06
            -4.500E-04    1.695E-09    7.510E-09   -2.315E-05   -1.896E-05   -1.210E-05    3.951E-07    1.173E-10   -1.164E-07    1.338E-09
            -2.859E-07   -1.842E-05    0.000E+00   -5.220E-05   -8.858E-05

 THE REACTION RATES ARE
        1.37E-02     1.55E-02     1.34E-02     1.25E-06     2.08E-07     7.52E-08     7.05E-05     1.68E-03     1.13E-04     1.02E-04
        1.18E-05     8.69E-07     3.18E-07     3.21E-06     6.53E-05     2.59E-09     8.01E-06     7.21E-08     7.93E-06     1.12E-08
        5.15E-11     1.23E-05     1.18E-05     1.59E-07     1.80E-13     6.21E-05     1.60E-07     1.91E-04     9.15E-05     9.14E-05
        1.61E-08     1.35E-08     1.01E-08     4.96E-10     3.25E-10     1.73E-05     1.94E-05     1.62E-05     2.63E-05     7.61E-09
        1.40E-09     1.92E-08     2.92E-05     5.27E-09     2.26E-06     2.83E-05     5.21E-05     3.98E-05     1.21E-10     3.16E-09
        3.18E-06     2.78E-05     1.30E-05     8.29E-06     4.79E-08     5.56E-08     1.60E-05     2.75E-06     5.07E-09     1.78E-08
        7.95E-06     7.27E-07     4.13E-06     1.80E-06     4.37E-06     3.92E-06     2.43E-06     4.00E-06     1.69E-06     7.07E-07
        9.45E-08     1.29E-05     1.68E-06     7.23E-06     0.00E+00     0.00E+00     0.00E+00     0.00E+00     1.07E-04     4.13E-06
        2.12E-09     3.17E-02     6.58E-06

 THE PHOTOLYTIC RATE CONSTANTS ARE
          5.467E-01    2.898E-02    1.959E-03    1.853E+01    1.080E-01    5.723E-04    1.858E-03    3.028E-03    2.741E-04
          1.560E-02    1.664E-02


 THE CURRENT MIXING HEIGHT IS     1119.47

 THE CURRENT TEMPERATURE IS        299.00

 THE CURRENT ZENITH ANGLE IS        30.10
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     TIME      NMOC        NMOC/        NOX         NO2          O3           NO2          MEOH
    (LDT )     TOTAL        NOX        TOTAL      FRACTION    (INSTANT)    (INSTANT)    (INSTANT)

    1200.      .25067     9.63161      .02603      .78662      .07281       .02047       .02380

  TIME        NO2         NO          O           O3          NO3         O1D         H2O         OH          HO2         N2O5
INTERVAL      HNO3        HNO2        PNA         H2O2        CO          FORM        ALD2        C2O3        XO2         PAN
              PAR         XO2N        ROR         OLE         ETH         TOL         CRES        TO2         OPEN        CRO
              MGLY        XYL         ISOP        NR          MEOH

 1.200E+03   2.047E-02   5.553E-03   3.381E-09   7.281E-02   2.791E-07   3.662E-10   1.500E+04   2.268E-07   3.486E-06   2.603E-06
 1.858E+01   8.179E-03   1.037E-04   1.959E-05   3.242E-06   3.385E-01   8.687E-03   7.369E-03   4.022E-07   2.015E-06   2.030E-03
             1.350E-01   9.928E-07   1.031E-10   1.440E-03   3.549E-03   2.457E-03   4.120E-04   2.029E-08   1.012E-04   1.469E-08
             3.993E-04   1.467E-03   0.000E+00   2.948E-02   2.380E-02

NET RATES   -7.909E-05  -4.227E-05  -1.911E-06   2.731E-04  -3.456E-08  -8.880E-09  -1.801E-05  -5.559E-08  -1.383E-07   1.349E-08
             6.100E-05  -1.521E-07   2.625E-07   6.992E-08  -2.525E-04   3.426E-06  -1.287E-05  -1.760E-07   2.546E-08   8.310E-06
            -2.687E-04   1.323E-08   1.971E-08  -1.565E-05  -1.426E-05  -8.502E-06  -1.095E-06   6.307E-10  -1.534E-07   6.112E-10
            -9.169E-07  -1.328E-05   0.000E+00  -2.648E-05  -4.908E-05

THE REACTION RATES ARE
        1.17E-02    1.41E-02    1.13E-02    9.52E-07    1.56E-07    4.49E-08    7.65E-05    2.20E-03    1.71E-04    1.53E-04
        1.79E-05    1.70E-06    7.76E-07    5.40E-06    6.79E-05    3.51E-09    1.05E-05    7.42E-08    1.04E-05    4.66E-09
        2.73E-11    1.20E-05    1.17E-05    2.30E-07    1.61E-13    7.62E-05    3.91E-07    2.36E-04    1.41E-04    1.41E-04
        3.00E-08    4.85E-08    3.27E-08    1.98E-09    1.86E-09    2.47E-05    2.95E-05    1.76E-05    2.81E-05    7.33E-09
        2.25E-09    1.64E-08    3.98E-05    7.61E-09    2.31E-06    4.06E-05    8.38E-05    7.20E-05    5.98E-10    1.35E-08
        5.04E-06    3.68E-05    1.85E-05    9.84E-06    4.64E-08    2.91E-08    1.35E-05    2.02E-06    4.56E-09    1.33E-08
        9.46E-06    7.62E-07    5.04E-06    1.35E-06    5.07E-06    5.70E-06    3.74E-06    6.02E-06    1.73E-06    1.01E-06
        1.12E-07    1.20E-05    2.35E-06    7.27E-06    0.00E+00    0.00E+00    0.00E+00    0.00E+00    1.34E-04    5.51E-06
        7.77E-09    2.95E-02    8.64E-06

THE PHOTOLYTIC RATE CONSTANTS ARE
        5.710E-01   3.026E-02   2.353E-03   1.936E+01   1.128E-01   6.117E-04   2.031E-03   3.236E-03   3.136E-04
        1.706E-02   1.820E-02


THE CURRENT MIXING HEIGHT IS      1340.22

THE CURRENT TEMPERATURE IS         301.00

THE CURRENT ZENITH ANGLE IS         20.18
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         TIME      NMOC       NMOC/        NOX         NO2          O3          NO2         MEOH
        (LDT )     TOTAL       NOX         TOTAL      FRACTION   (INSTANT)   (INSTANT)   (INSTANT)

        1300.     .21948    11.64461      .01885      .82757      .09108      .01560      .02135

  TIME        NO2         NO          O           O3          NO3         O1D         H2O         OH          HO2         N2O5
 INTERVAL     HNO3        HNO2        PNA         H2O2        CO          FORM        ALD2        C2O3        XO2         PAN
              PAR         XO2N        ROR         OLE         ETH         TOL         CRES        TO2         OPEN        CRO
              MGLY        XYL         ISOP        NR          MEOH

 1.300E+03   1.560E-02   3.250E-03   2.972E-09   9.108E-02   4.541E-07   4.914E-10   1.500E+04   3.402E-07   7.357E-06   2.539E-06
 1.858E+01   1.221E-02   8.972E-05   2.492E-05   1.276E-05   3.280E-01   8.968E-03   6.556E-03   9.228E-07   4.257E-06   2.488E-03
             1.209E-01   2.287E-06   1.234E-10   6.777E-04   2.733E-03   1.978E-03   3.124E-04   2.165E-08   8.635E-05   2.309E-08
             3.215E-04   7.821E-04   0.000E+00   2.824E-02   2.135E-02

NET RATES   -8.528E-05  -3.161E-05   2.663E-06   3.392E-04   5.440E-08   1.491E-08  -2.423E-05  -3.946E-07   1.067E-06  -2.451E-08
             7.182E-05  -3.332E-07  -4.353E-07   3.012E-07  -1.162E-04   4.491E-06  -1.458E-05   4.142E-07   2.795E-07   7.006E-06
            -2.124E-04   4.960E-08  -3.917E-08  -9.739E-06  -1.311E-05  -7.634E-06  -2.048E-06   1.417E-09  -3.549E-07   9.882E-10
            -1.668E-06  -9.474E-06   0.000E+00  -1.562E-05  -3.455E-05

THE REACTION RATES ARE
     9.04E-03     1.20E-02     8.51E-03     6.38E-07     1.03E-07     2.28E-08     7.70E-05     2.80E-03     2.28E-04     2.04E-04
     2.40E-05     3.26E-06     2.08E-06     8.92E-06     6.43E-05     4.47E-09     1.29E-05     7.24E-08     1.29E-05     1.58E-09
     1.22E-11     1.04E-05     1.03E-05     2.98E-07     1.21E-13     8.58E-05     8.56E-07     2.90E-04     2.23E-04     2.23E-04
     5.67E-08     2.10E-07     1.28E-07     7.97E-09     1.11E-08     3.59E-05     4.58E-05     1.88E-05     2.96E-05     6.88E-09
     3.79E-09     1.31E-08     5.28E-05     1.10E-08     2.15E-06     5.42E-05     1.30E-04     1.20E-04     3.15E-09     6.52E-08
     7.85E-06     4.95E-05     2.63E-05     1.18E-05     4.23E-08     1.21E-08     9.42E-06     1.25E-06     3.49E-09     9.17E-09
     1.08E-05     7.78E-07     6.05E-06     8.44E-07     5.41E-06     6.48E-06     4.61E-06     7.20E-06     1.52E-06     1.29E-06
     1.21E-07     9.57E-06     2.84E-06     6.03E-06     0.00E+00     0.00E+00     0.00E+00     0.00E+00     1.66E-04     7.43E-06
     3.37E-08     2.82E-02     1.16E-05

THE PHOTOLYTIC RATE CONSTANTS ARE
       5.793E-01    3.070E-02    2.506E-03    1.964E+01    1.144E-01    6.247E-04    2.094E-03    3.305E-03    3.278E-04
       1.759E-02    1.876E-02


THE CURRENT MIXING HEIGHT IS     1496.21

THE CURRENT TEMPERATURE IS        303.00

THE CURRENT ZENITH ANGLE IS        15.19
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      TIME      NMOC       NMOC/        NOX          NO2         O3          NO2         MEOH
     (LDT )     TOTAL       NOX         TOTAL      FRACTION   (INSTANT)   (INSTANT)   (INSTANT)

     1400.      .19359    16.07089      .01205       .86496      .11301      .01042      .01945

   TIME        NO2         NO          O           O3          NO3         O1D         H2O         OH          HO2         N2O5
 INTERVAL      HNO3        HNO2        PNA         H2O2        CO          FORM        ALD2        C2O3        XO2         PAN
               PAR         XO2N        ROR         OLE         ETH         TOL         CRES        TO2         OPEN        CRO
               MGLY        XYL         ISOP        NR          MEOH

 1.400E+03   1.042E-02   1.627E-03   2.413E-09   1.130E-01   6.972E-07   5.805E-10   1.500E+04   4.804E-07   1.680E-05   2.291E-06
 1.491E+01   1.642E-02   6.490E-05   3.351E-05   5.806E-05   3.230E-01   8.981E-03   5.604E-03   2.055E-06   9.606E-06   2.999E-03
             1.086E-01   5.793E-06   1.467E-10   2.573E-04   1.976E-03   1.531E-03   1.944E-04   2.020E-08   6.100E-05   3.207E-08
             2.084E-04   3.391E-04   0.000E+00   2.747E-02   1.945E-02

 NET RATES  -8.964E-05  -1.722E-05  -7.253E-06   3.980E-04  -1.720E-07  -5.857E-08  -2.908E-05  -1.519E-07  -1.916E-06   7.627E-08
             6.626E-05  -4.468E-07   2.211E-06   1.547E-06  -5.529E-05  -3.535E-06  -1.657E-05  -1.802E-06   4.591E-08   1.102E-05
            -1.977E-04   9.438E-08   1.626E-07  -4.461E-06  -1.193E-05  -7.194E-06  -1.709E-06  -3.428E-10  -4.416E-07  -5.525E-10
            -1.927E-06  -5.269E-06   0.000E+00  -9.904E-06  -2.874E-05

 THE REACTION RATES ARE
       5.96E-03    9.65E-03    5.36E-03    3.46E-07    5.55E-08    9.19E-09    6.55E-05    3.43E-03    2.69E-04    2.40E-04
       2.84E-05    5.78E-06    5.92E-06    1.35E-05    4.93E-05    4.65E-09    1.32E-05    6.53E-08    1.31E-05    3.93E-10
       4.07E-12    7.26E-06    7.33E-06    3.05E-07    6.32E-14    8.03E-05    1.61E-06    3.30E-04    3.37E-04    3.35E-04
       1.07E-07    1.08E-06    6.29E-07    3.56E-08    7.12E-08    5.00E-05    6.47E-05    1.83E-05    2.92E-05    5.69E-09
       5.82E-09    9.18E-09    6.35E-05    1.45E-08    1.77E-06    6.02E-05    1.82E-04    1.68E-04    1.56E-08    3.31E-07
       1.13E-05    6.28E-05    3.42E-05    1.40E-05    3.36E-08    3.76E-09    5.02E-06    6.02E-07    2.04E-09    5.43E-09
       1.10E-05    7.18E-07    6.59E-06    3.94E-07    5.05E-06    5.70E-06    4.40E-06    6.68E-06    1.05E-06    1.29E-06
       1.07E-07    5.85E-06    2.60E-06    3.81E-06    0.00E+00    0.00E+00    0.00E+00    0.00E+00    1.88E-04    9.42E-06
       1.69E-07    2.75E-02    1.49E-05

 THE PHOTOLYTIC RATE CONSTANTS ARE
       5.722E-01   3.033E-02   2.376E-03   1.940E+01   1.130E-01   6.137E-04   2.041E-03   3.247E-03   3.158E-04
       1.714E-02   1.828E-02


 THE CURRENT MIXING HEIGHT IS     1610.77

 THE CURRENT TEMPERATURE IS        304.00

 THE CURRENT ZENITH ANGLE IS        19.50
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        TIME     NMOC      NMOC/       NOX         NO2         O3        NO2        MEOH
       (LDT )    TOTAL      NOX        TOTAL     FRACTION  (INSTANT)  (INSTANT)  (INSTANT)

       1500.    .17121   24.95541     .00686      .90174     .13718     .00619     .01781

  TIME         NO2         NO          O           O3          NO3         O1D         H2O         OH          HO2         N2O5
INTERVAL       HNO3        HNO2        PNA         H2O2        CO          FORM        ALD2        C2O3        XO2         PAN
               PAR         XO2N        ROR         OLE         ETH         TOL         CRES        TO2         OPEN        CRO
               MGLY        XYL         ISOP        NR          MEOH

 1.500E+03   6.187E-03   6.741E-04   1.963E-09   1.372E-01   1.016E-06   5.975E-10   1.500E+04   6.184E-07   4.186E-05   1.572E-06
 1.037E+01   1.989E-02   3.700E-05   3.949E-05   3.256E-04   3.206E-01   8.724E-03   4.688E-03   5.540E-06   2.517E-05   3.362E-03
             9.665E-02   1.596E-05   1.490E-10   9.149E-05   1.319E-03   1.120E-03   1.115E-04   1.659E-08   3.741E-05   4.335E-08
             1.069E-04   1.249E-04   0.000E+00   2.699E-02   1.781E-02

NET RATES   -5.668E-05  -1.026E-05  -2.762E-10   3.936E-04   4.827E-09   2.910E-11  -3.271E-05   1.033E-09   5.093E-07  -1.261E-08
             4.613E-05  -4.614E-07  -4.922E-09   9.050E-06  -2.873E-05  -5.400E-06  -1.349E-05   8.143E-08   3.462E-07   1.558E-06
            -1.976E-04   2.263E-07  -2.734E-12  -1.458E-06  -9.554E-06  -6.250E-06  -1.056E-06  -1.034E-10  -3.349E-07   1.505E-10
            -1.371E-06  -2.097E-06   0.000E+00  -6.814E-06  -2.636E-05

THE REACTION RATES ARE
        3.40E-03     7.65E-03     2.78E-03     1.67E-07     2.64E-08     3.06E-09     4.98E-05     3.99E-03     2.74E-04     2.45E-04
        2.92E-05     9.21E-06     1.81E-05     1.89E-05     2.96E-05     4.13E-09     1.14E-05     4.48E-08     1.14E-05     6.68E-11
        1.00E-12     3.81E-06     4.01E-06     2.24E-07     2.05E-14     6.04E-05     2.45E-06     3.39E-04     4.91E-04     4.91E-04
        1.61E-07     6.56E-06     3.45E-06     1.88E-07     5.16E-07     6.38E-05     8.09E-05     1.64E-05     2.66E-05     4.65E-09
        8.24E-09     6.38E-09     6.81E-05     1.76E-08     1.30E-06     6.69E-05     2.59E-04     2.55E-04     1.14E-07     2.23E-06
        1.51E-05     7.19E-05     4.12E-05     1.42E-05     2.03E-08     1.09E-09     2.27E-06     2.72E-07     1.05E-09     3.00E-09
        9.38E-06     6.16E-07     6.16E-06     1.34E-07     4.15E-06     4.21E-06     3.68E-06     5.36E-06     5.90E-07     1.02E-06
        8.04E-08     2.77E-06     1.72E-06     1.80E-06     0.00E+00     0.00E+00     0.00E+00     0.00E+00     2.04E-04     1.08E-05
        1.13E-06     2.70E-02     1.76E-05

THE PHOTOLYTIC RATE CONSTANTS ARE
          5.494E-01   2.912E-02   2.000E-03   1.862E+01   1.085E-01   5.766E-04   1.877E-03   3.051E-03   2.783E-04
          1.577E-02   1.682E-02


THE CURRENT MIXING HEIGHT IS     1700.00

THE CURRENT TEMPERATURE IS        306.00

THE CURRENT ZENITH ANGLE IS        29.20
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     TIME       NMOC       NMOC/       NOX        NO2         O3          NO2         MEOH
    (LDT )      TOTAL       NOX        TOTAL     FRACTION   (INSTANT)   (INSTANT)   (INSTANT)

    1600.      .15809    38.78848     .00408     .92322      .15774      .00376      .01708

  TIME         NO2         NO          O           O3          NO3         O1D         H2O         OH          HO2         N2O5
 INTERVAL      HNO3        HNO2        PNA         H2O2        CO          FORM        ALD2        C2O3        XO2         PAN
               PAR         XO2N        ROR         OLE         ETH         TOL         CRES        TO2         OPEN        CRO
               MGLY        XYL         ISOP        NR          MEOH

 1.600E+03   3.763E-03   3.129E-04   1.633E-09   1.577E-01   1.128E-06   4.935E-10   1.500E+04   5.120E-07   5.940E-05   1.061E-06
 1.352E+01   2.257E-02   1.592E-05   3.409E-05   1.204E-03   3.243E-01   8.389E-03   4.144E-03   8.872E-06   3.973E-05   3.365E-03
             8.893E-02   2.653E-05   1.136E-10   3.901E-05   8.922E-04   8.473E-04   6.684E-05   9.716E-09   2.218E-05   4.365E-08
             5.060E-05   5.533E-05   0.000E+00   2.716E-02   1.708E-02

NET RATES   -2.311E-05  -3.503E-06  -2.251E-07   2.396E-04  -3.934E-09   3.436E-09  -3.110E-05   1.147E-07  -2.268E-07  -2.896E-09
             3.067E-05  -2.113E-07   3.064E-08   1.796E-05   5.020E-05  -7.807E-06  -7.135E-06  -1.961E-07   1.928E-08  -3.130E-06
            -1.046E-04   7.616E-08   5.047E-09  -2.551E-07  -5.013E-06  -3.364E-06  -5.160E-07   1.073E-10  -1.906E-07  -2.622E-10
            -5.692E-07  -4.456E-07   0.000E+00   3.271E-06  -9.665E-06

THE REACTION RATES ARE
      1.91E-03    6.37E-03    1.48E-03    8.45E-08    1.34E-08    1.18E-09    3.48E-05    4.24E-03    2.27E-04    2.03E-04
      2.41E-05    8.77E-06    2.96E-05    1.94E-05    1.52E-05    2.79E-09    7.69E-06    3.02E-08    7.66E-06    1.44E-11
      2.83E-13    1.46E-06    1.59E-06    7.96E-08    3.80E-15    3.04E-05    2.31E-06    2.23E-04    4.24E-04    4.24E-04
      1.15E-07    1.32E-05    6.94E-06    6.16E-07    1.58E-06    5.35E-05    6.44E-05    1.33E-05    2.27E-05    3.72E-09
      8.80E-09    4.69E-09    4.98E-05    1.73E-08    9.07E-07    4.97E-05    2.52E-04    2.55E-04    2.91E-07    5.06E-06
      1.25E-05    5.48E-05    3.14E-05    1.08E-05    9.40E-09    3.88E-10    8.03E-07    1.33E-07    4.99E-10    1.69E-09
      5.25E-06    4.79E-07    3.86E-06    3.65E-08    2.43E-06    2.09E-06    2.45E-06    3.28E-06    2.95E-07    5.00E-07
      5.48E-08    1.02E-06    6.74E-07    7.19E-07    0.00E+00    0.00E+00    0.00E+00    0.00E+00    1.49E-04    8.30E-06
      2.82E-06    2.72E-02    1.40E-05

THE PHOTOLYTIC RATE CONSTANTS ARE
      5.071E-01    2.688E-02   1.437E-03   1.719E+01   1.002E-01   5.118E-04   1.585E-03   2.708E-03   2.188E-04
      1.331E-02    1.420E-02


THE CURRENT MIXING HEIGHT IS     1701.34

THE CURRENT TEMPERATURE IS        306.00

THE CURRENT ZENITH ANGLE IS        40.48
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        TIME      NMOC        NMOC/         NOX          NO2         O3          NO2          MEOH
       (LDT )     TOTAL        NOX         TOTAL       FRACTION   (INSTANT)   (INSTANT)    (INSTANT)

      1700.      .15034     47.56795      .00316       .93352      .16698      .00295       .01665

   TIME          NO2          NO           O            O3           NO3          O1D          H2O          OH           HO2          N2O5
 INTERVAL        HNO3         HNO2         PNA          H2O2         CO           FORM         ALD2         C2O3         XO2          PAN
                 PAR          XO2N         ROR          OLE          ETH          TOL          CRES         TO2          OPEN         CRO
                 MGLY         XYL          ISOP         NR           MEOH

 1.700E+03    2.950E-03    2.101E-04    1.347E-09    1.670E-01    1.172E-06    3.019E-10    1.500E+04    3.460E-07    5.227E-05    9.717E-07
 1.352E+01    2.391E-02    8.230E-06    2.639E-05    2.186E-03    3.267E-01    7.904E-03    3.814E-03    8.427E-06    3.717E-05    3.107E-03
              8.410E-02    2.584E-05    7.720E-11    3.562E-05    6.796E-04    7.008E-04    4.339E-05    5.467E-09    1.388E-05    3.424E-08
              3.107E-05    4.528E-05    0.000E+00    2.736E-02    1.665E-02

NET RATES    -6.298E-06   -1.909E-07   -1.111E-06    8.450E-05    2.037E-09   -1.714E-08   -2.051E-05   -1.160E-07   -6.256E-07    1.141E-08
              1.632E-05   -7.152E-08    3.632E-07    1.324E-05    3.302E-05   -7.671E-06   -3.976E-06   -7.930E-07   -1.942E-07   -3.693E-06
             -5.596E-05   -9.422E-08    2.658E-08    1.221E-07   -2.303E-06   -1.622E-06   -3.103E-07    1.980E-10   -9.891E-08   -1.072E-09
             -1.537E-07    6.189E-08    0.000E+00    3.584E-06   -4.475E-06

THE REACTION RATES ARE
     1.29E-03     5.32E-03     1.04E-03     5.46E-08     8.70E-09     6.59E-10     2.81E-05     3.88E-03     1.39E-04     1.24E-04
     1.48E-05     6.21E-06     2.74E-05     1.74E-05     1.07E-05     2.24E-09     6.28E-06     2.77E-08     6.24E-06     6.52E-12
     1.49E-13     6.70E-07     7.13E-07     2.78E-08     1.02E-15     1.63E-05     1.67E-06     1.32E-04     2.95E-04     2.94E-04
     6.06E-08     1.04E-05     5.72E-06     9.05E-07     1.93E-06     3.64E-05     4.10E-05     9.40E-06     1.73E-05     2.84E-09
     8.62E-09     3.53E-09     3.11E-05     1.65E-08     5.61E-07     3.18E-05     1.99E-04     2.03E-04     2.63E-07     4.23E-06
     8.29E-06     3.50E-05     1.96E-05     7.37E-06     5.01E-09     2.91E-10     4.98E-07     1.26E-07     4.74E-10     1.05E-09
     2.72E-06     3.76E-07     2.16E-06     1.38E-08     1.37E-06     9.16E-07     1.65E-06     2.02E-06     1.39E-07     2.11E-07
     3.61E-08     5.62E-07     2.79E-07     3.31E-07     0.00E+00     0.00E+00     0.00E+00     0.00E+00     9.37E-05     5.43E-06
     2.50E-06     2.74E-02     9.22E-06

THE PHOTOLYTIC RATE CONSTANTS ARE
        4.388E-01    2.326E-02    8.334E-04    1.488E+01    8.667E-02    4.140E-04    1.189E-03    2.191E-03    1.470E-04
        9.991E-03    1.066E-02


THE CURRENT MIXING HEIGHT IS     1701.34

THE CURRENT TEMPERATURE IS        305.00

THE CURRENT ZENITH ANGLE IS        52.16
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   TIME       NMOC        NMOC/          NOX          NO2         O3          NO2          MEOH
  (LDT )      TOTAL        NOX          TOTAL      FRACTION   (INSTANT)   (INSTANT)    (INSTANT)

  1800.      .14717     45.41303       .00324       .94491      .16912      .00306       .01653

 TIME          NO2         NO          O           O3          NO3         O1D         H2O         OH          HO2         N2O5
INTERVAL       HNO3        HNO2        PNA         H2O2        CO          FORM        ALD2        C2O3        XO2         PAN
               PAR         XO2N        ROR         OLE         ETH         TOL         CRES        TO2         OPEN        CRO
               MGLY        XYL         ISOP        NR          MEOH

 1.800E+03  3.062E-03   1.785E-04   1.024E-09   1.691E-01   1.488E-06   1.159E-10   1.500E+04   1.965E-07   3.505E-05   1.447E-06
 1.537E+01  2.469E-02   5.378E-06   2.074E-05   2.737E-03   3.283E-01   7.547E-03   3.658E-03   5.955E-06   2.491E-05   2.845E-03
            8.198E-02   1.734E-05   4.555E-11   4.845E-05   5.916E-04   6.392E-04   2.578E-05   2.977E-09   9.246E-06   2.237E-08
            2.782E-05   5.707E-05   0.000E+00   2.760E-02   1.653E-02

NET RATES   5.753E-06  -1.169E-06   4.924E-07   1.040E-04   4.803E-08   4.512E-09  -8.444E-06  -4.899E-09   1.854E-07  -6.970E-09
            1.002E-05  -4.073E-08  -6.128E-07   5.308E-06   1.907E-05  -4.093E-06  -1.754E-06   7.172E-07  -2.341E-07  -4.673E-06
           -2.361E-05  -1.526E-07  -1.754E-08   7.221E-08  -1.005E-06  -6.677E-07  -3.253E-07   2.424E-10  -6.151E-08  -3.104E-10
            6.021E-09   1.233E-07   0.000E+00   3.023E-06  -1.198E-06

THE REACTION RATES ARE
     1.03E-03     4.10E-03     8.81E-04     4.31E-08     6.92E-09     4.28E-10     2.88E-05     3.01E-03     5.36E-05     4.79E-05
     5.67E-06     3.54E-06     1.85E-05     1.69E-05     1.15E-05     2.92E-09     8.30E-06     4.12E-08     8.26E-06     4.74E-12
     1.31E-13     3.26E-07     3.56E-07     1.03E-08     4.34E-16     9.65E-06     9.89E-07     7.56E-05     2.07E-04     2.07E-04
     2.72E-08     4.72E-06     2.74E-06     7.74E-07     1.37E-06     2.08E-05     2.22E-05     5.42E-06     1.13E-05     2.03E-09
     1.04E-08     2.54E-09     1.70E-05     2.01E-08     2.69E-07     1.92E-05     1.55E-04     1.60E-04     1.31E-07     2.00E-06
     4.62E-06     1.94E-05     1.06E-05     4.35E-06     3.07E-09     3.00E-10     3.87E-07     1.70E-07     8.18E-10     6.90E-10
     1.35E-06     3.22E-07     1.13E-06     6.38E-09     7.44E-07     3.09E-07     1.25E-06     1.37E-06     5.58E-08     7.99E-08
     2.42E-08     4.03E-07     1.42E-07     1.79E-07     0.00E+00     0.00E+00     0.00E+00     0.00E+00     5.34E-05     3.10E-06
     1.14E-06     2.76E-02     5.20E-06

THE PHOTOLYTIC RATE CONSTANTS ARE
        3.355E-01    1.778E-02    3.170E-04    1.137E+01    6.625E-02    2.828E-04    7.181E-04    1.496E-03    7.366E-05
        6.032E-03    6.434E-03


THE CURRENT MIXING HEIGHT IS     1701.34

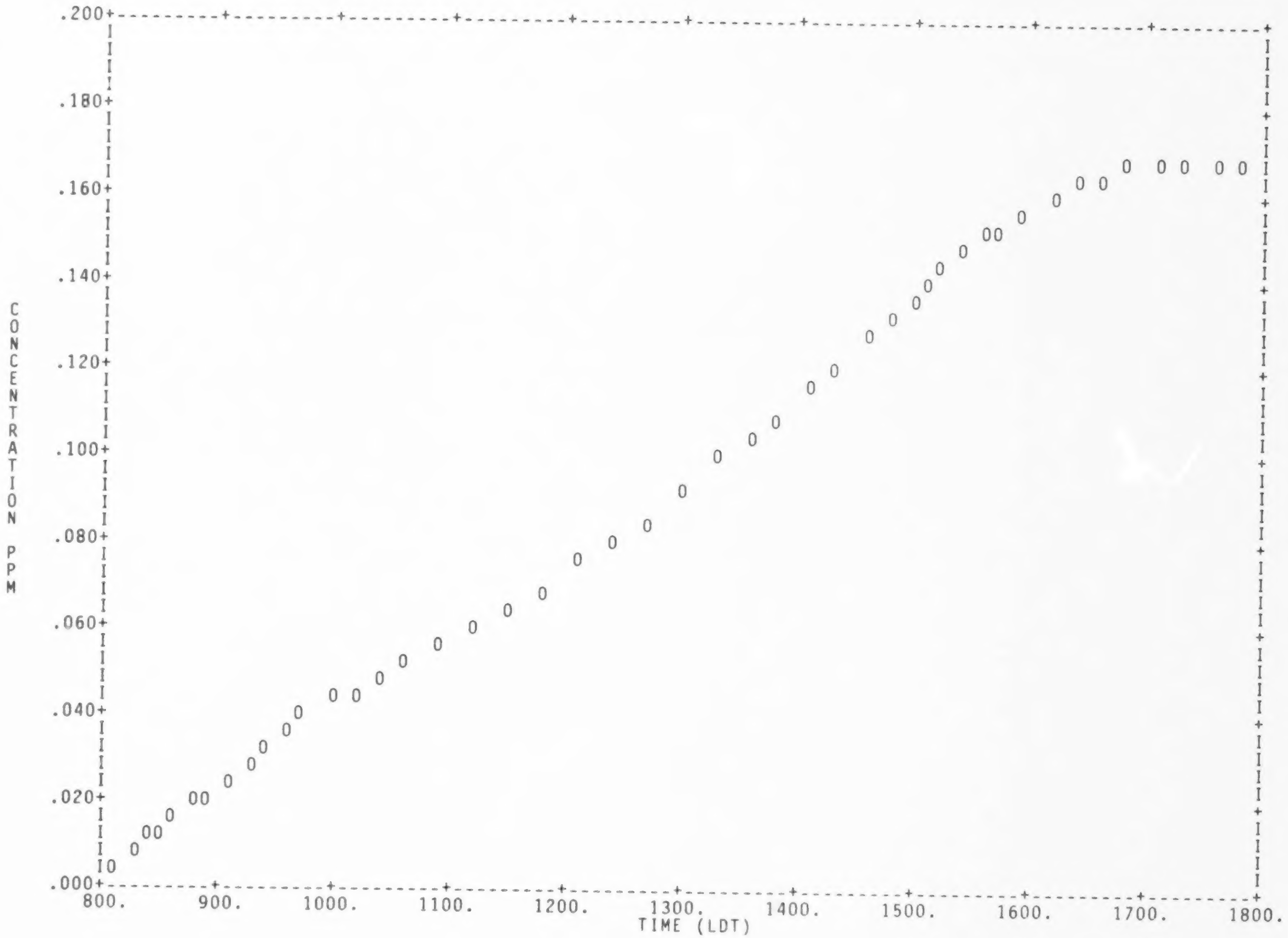
THE CURRENT TEMPERATURE IS        304.00

THE CURRENT ZENITH ANGLE IS        63.80
```

```
MAXIMUM O3    NOT REACHED, THE LAST ONE HOUR AVERAGE WAS  .16788 PPM.

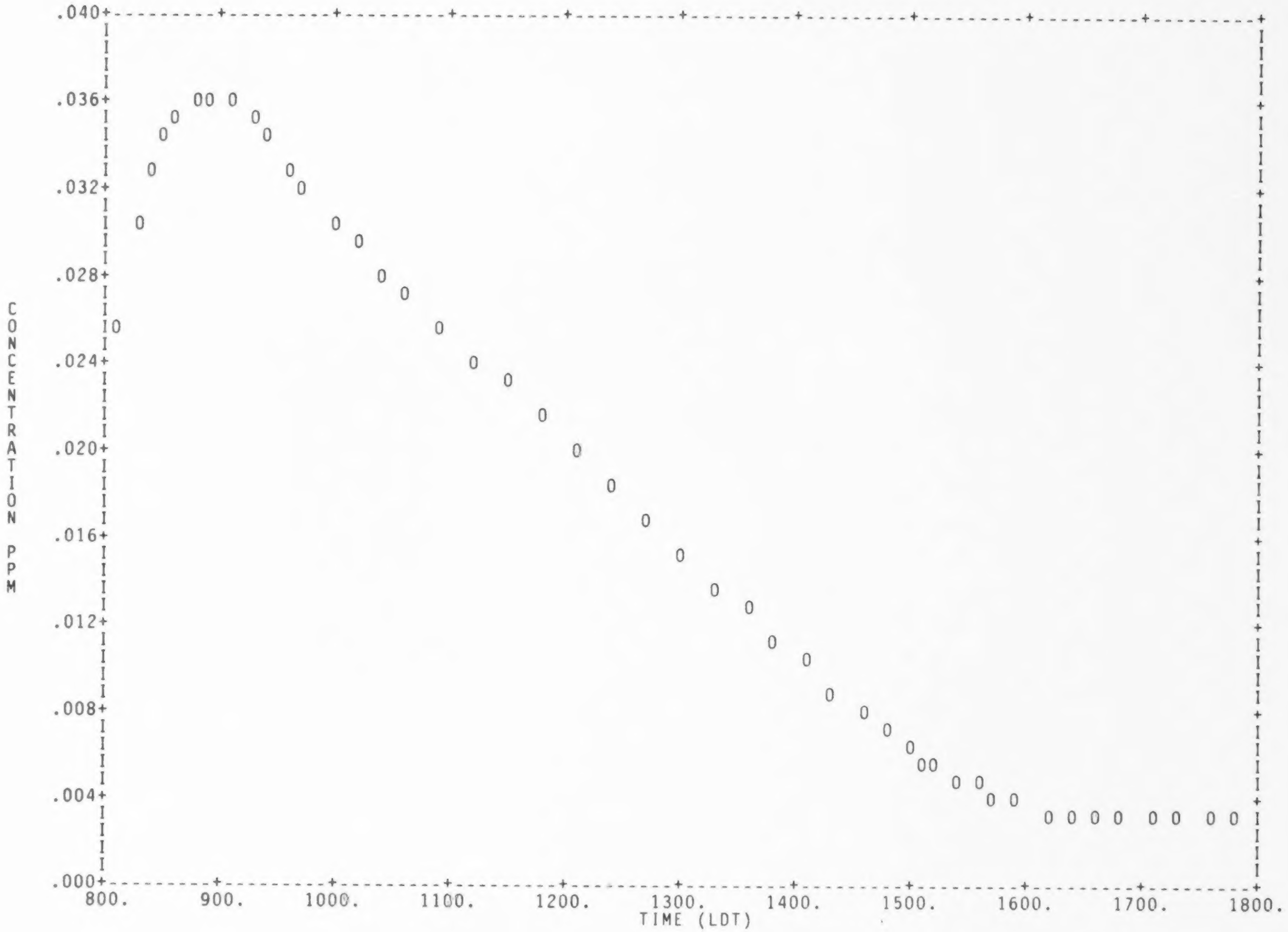
MAXIMUM ONE HOUR AVE NO2   =  .03540 CENTERED AT  859. LDT

MAXIMUM ONE HOUR AVE MEOH  =  .07392 CENTERED AT  830. LDT
```



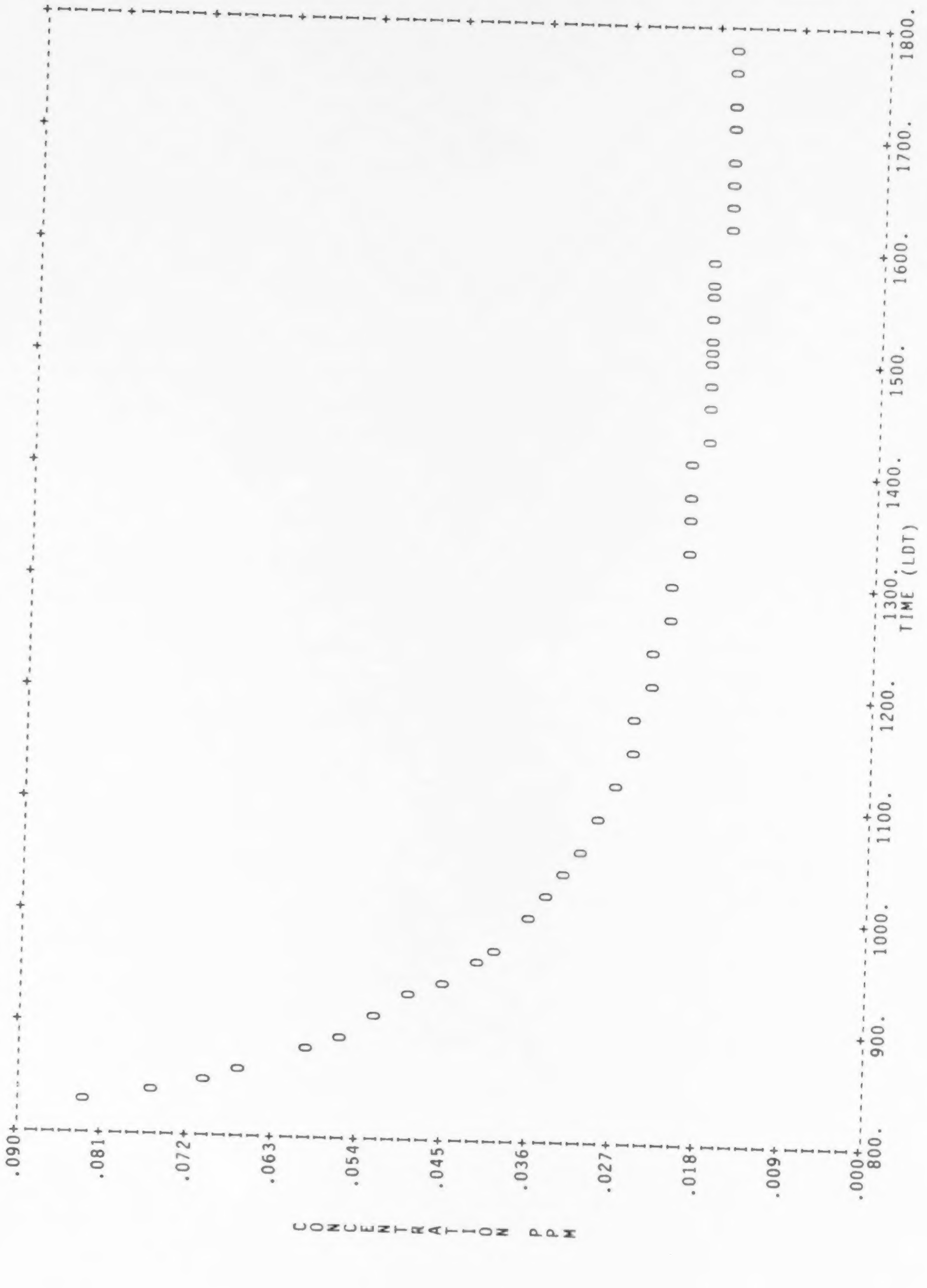
EXAMPLE 2 - CB4 WITH METHANOL REACTION ADDED

03 CONCENTRATION AS A FUNCTION OF TIME



EXAMPLE 2 - CB4 WITH METHANOL REACTION ADDED

NO2 CONCENTRATION AS A FUNCTION OF TIME



EXAMPLE 2 - CB4 WITH METHANOL REACTION ADDED

MEOH CONCENTRATION AS A FUNCTION OF TIME

EXHIBIT 5

```
(    1)          1         2         3         4         5         6         7
(    2) 123456789012345678901234567890123456789012345678901234567890123456789012
(    3)
(    4) TITL
(    5) EXAMPLE 3 - EKMA OPTION USING MASS AND CREDIT OPTIONS
(    6) TRANS     .060      .080      0.        .050      0.        0.009
(    7) PLAC      38.629    90.206    5.0       1986.     6.0       21.
(    8) TEST CITY
(    9) DILU      250.      1700.
(   10) MASS      -11.      .6        0.05      250.
(   11) 9.42      7.68      7.54      5.21      3.23      2.24      2.18
(   12) 1.75      1.72      2.10      1.12
(   13) 8.11      6.18      5.65      4.11      2.76      1.90      1.91
(   14) 1.60      1.42      1.78      0.90
(   15) CRED                -11.       250.
(   16) CO        1.                  .5        -35.                .5
(   17) 12.9      19.4      14.2      11.6      11.6      11.6      11.6
(   18) 12.9      14.2      15.5      20.7
(   19) EKMA      .17       10.       -10.      1.        2.        1.
(   20) -1.       -1.       0.        0.04      0.        0.009
(   21) .6        .05                           -50.
(   22)     BLANK
(   23)
(   24)          1         2         3         4         5         6         7
(   25) 123456789012345678901234567890123456789012345678901234567890123456789012
```

```
***************************************
*                                     *
*   OZONE ISOPLETH PLOTTING PACKAGE   *
*      WITH OPTIONAL MECHANISMS       *
*                                     *
*              O Z I P M              *
*                                     *
*             VERSION 4.00            *
*                                     *
*            DECEMBER, 1987           *
*                                     *
***************************************
```

EXHIBIT 6

```
THE INPUTS FOR THIS RUN ARE


         TITL
         EXAMPLE 3 - EKMA OPTION USING MASS AND CREDIT OPTIONS
         TRANS     .060      .080      0.        .050      0.        0.009
         PLAC      38.629    90.206    5.0       1986.     6.0       21.
         TEST CITY
         DILU      250.      1700.
         MASS      -11.      .6        0.05      250.
         9.42      7.68      7.54      5.21      3.23      2.24      2.18
         1.75      1.72      2.10      1.12
         8.11      6.18      5.65      4.11      2.76      1.90      1.91
         1.60      1.42      1.78      0.90
         CRED                -11.       250.
         CO        1.                  .5        -35.                .5
         12.9      19.4      14.2      11.6      11.6      11.6      11.6
         12.9      14.2      15.5      20.7
         EKMA      .17       10.       -10.      1.        2.        1.
         -1.       -1.       0.        0.04      0.        0.009
         .6        .05                           -50.
             BLANK
```

```
EXAMPLE 3 - EKMA OPTION USING MASS AND CREDIT OPTIONS

PHOTOLYTIC RATE CONSTANTS CALCULATED FOR

         TEST CITY

LATITUDE      38.629
LONGITUDE     90.206
TIME ZONE     5.0
DATE          6      21    1986
TIME          800    TO    1800     LOCAL DAYLIGHT TIME


DILUTION DETERMINED FROM THE FOLLOWING
INVERSION HEIGHTS      INITIAL    250.     FINAL      1700.
TIMING                 START      800.     STOP       1500.


MIXING HEIGHTS (AT THE BEGINNING OF EACH HOUR)
TIME       800      900     1000     1100     1200     1300     1400     1500

HEIGHT     250.0    503.1   821.2   1119.5   1340.2   1496.2   1610.8   1700.0

REACTIVITY

EMISSIONS        ETH  FRACTION  .037   OLE  FRACTION  .035   ALD2 FRACTION  .052

EMISSIONS        FORM FRACTION  .021   TOL  FRACTION  .089   XYL  FRACTION  .117

EMISSIONS        PAR  FRACTION  .564   ISOP FRACTION  .000   NR   FRACTION  .085

ALOFT            ETH  FRACTION  .034   OLE  FRACTION  .020   ALD2 FRACTION  .037

ALOFT            FORM FRACTION  .070   TOL  FRACTION  .042   XYL  FRACTION  .026

ALOFT            PAR  FRACTION  .498   ISOP FRACTION  .000   NR   FRACTION  .273

NO2/NOX        .250
```

```
TRANSPORTED CONCENTRATIONS
SURFACE LAYER       OZONE     .060      HYDROCARBON   .000    NOX       .000 PPM
ALOFT               OZONE     .080      HYDROCARBON   .050    NOX       .009 PPM

CONTINUOUS EMISSIONS (EXPRESSED AS FRACTION OF THE INITIAL PRECURSORS)
SPECIES     HOUR          1     2     3     4     5     6     7     8     9    10
                         11

 VOC      FRACTION      .106  .086  .084  .058  .036  .025  .024  .020  .019  .024
                        .013

 NOX      FRACTION      .343  .262  .239  .174  .117  .080  .081  .068  .060  .075
                        .038

 CO       FRACTION      .045  .068  .050  .041  .041  .041  .041  .045  .050  .054
                        .072
```

```
EKMA CALCULATIONS ARE PERFORMED TO ESTIMATE

SITE-SPECIFIC VOC CONTROL REQUIREMENTS

BASE YEAR OZONE                            .170 PPM

BASE YEAR NMOC/NOX                       10.000

ANTICIPATED CHANGE IN NOX               -10.000 PERCENT

FUTURE OZONE TRANSPORTED ALOFT             .068 PPM

FUTURE NMOC TRANSPORTED ALOFT              .040 PPMC

FUTURE NOX TRANSPORTED ALOFT               .009 PPM

EMISSION CREDITS WILL BE ALLOWED FOR CO

ANTICIPATED CHANGE IN CO                -35.000 PERCENT

FUTURE CO   TRANSPORTED ALOFT              .500 PPM

FUTURE OZONE IN THE SURFACE LAYER          .054 PPM

FUTURE NMOC IN THE SURFACE LAYER           .000 PPMC

FUTURE NOX IN THE SURFACE LAYER            .000 PPM
```

```
                     THE FOLLOWING SIMULATIONS WERE DONE.

     NMOC            NOX             RATIO            O3              TIME

   1.00000          .10000         10.00000         .20996          NOT MAX

    .80967          .08097         10.00000         .19767          NOT MAX

    .38139          .03814         10.00000         .16372          NOT MAX

    .46065          .04607         10.00000         .17082          NOT MAX

    .23033          .04146          5.55556         .13423          NOT MAX

    .20591          .04146          4.96660         .13056          NOT MAX

    .13567          .04146          3.27243         .11759          NOT MAX

    .14872          .04146          3.58727         .12032          NOT MAX

                     VOC CONTROL REQUIREMENT IS  67.7 PERCENT
```

```
                    THE FOLLOWING SIMULATION WAS DONE WITH A

                     -50.00 PERCENT CHANGE IN NMOC.

   NMOC            NOX            RATIO            O3            TIME

  .23033         .04146          5.55556         .13423         NOT MAX
```

```
EKMA PREDICTED CHANGES IN OZONE

HC      NOX      O3     %-CHG HC   %-CHG NOX   %-CHG O3

.461    .041    .1591        .0      -10.0        -6.4
.415    .041    .1551     -10.0      -10.0        -8.8
.369    .041    .1508     -20.0      -10.0       -11.3
.322    .041    .1459     -30.0      -10.0       -14.2
.276    .041    .1405     -40.0      -10.0       -17.3
.230    .041    .1342     -50.0      -10.0       -21.0
.184    .041    .1270     -60.0      -10.0       -25.3
.138    .041    .1181     -70.0      -10.0       -30.5
.092    .041    .1073     -80.0      -10.0       -36.9
.046    .041    .0954     -90.0      -10.0       -43.9
.000    .041    .0846    -100.0      -10.0       -50.2
```

EXHIBIT 7

```
         1         2         3         4         5         6         7
123456789012345678901234567890123456789012345678901234567890123456789012

TITL
EXAMPLE 4 - EKMA OPTION - 1981 APPENDIX B PROCEDURES
TRANS     .060      .100      0.08      .09       0.        0.009
PLAC      38.629    90.206    5.0       1986.     6.0       21.
TEST CITY
DILU      250.      1700.
MASS      -11.      .6        0.05      250.
9.42      7.68      7.54      5.21      3.23      2.24      2.18
1.75      1.72      2.10      1.12
8.11      6.18      5.65      4.11      2.76      1.90      1.91
1.60      1.42      1.78      0.90
CRED                -11.       250.
CO        1.                  .5        -35.                .5
12.9      19.4      14.2      11.6      11.6      11.6      11.6
12.9      14.2      15.5      20.7
EKMA      .17       10.       -10.      1.
-1.       -1.       -.32      0.05      0.        0.009
.6        .05
    BLANK

         1         2         3         4         5         6         7
123456789012345678901234567890123456789012345678901234567890123456789012
```

```
*************************************
*                                   *
*  OZONE ISOPLETH PLOTTING PACKAGE  *
*     WITH OPTIONAL MECHANISMS      *
*                                   *
*            O Z I P M              *
*                                   *
*          VERSION 4.00             *
*                                   *
*         DECEMBER, 1987            *
*                                   *
*************************************
```

EXHIBIT 8

```
THE INPUTS FOR THIS RUN ARE

         TITL
         EXAMPLE 4 - EKMA OPTION - 1981 APPENDIX B PROCEDURES
         TRANS     .060      .100      0.08      .09       0.        0.009
         PLAC      38.629    90.206    5.0       1986.     6.0       21.
         TEST CITY
         DILU      250.      1700.
         MASS      -11.      .6        0.05      250.
         9.42      7.68      7.54      5.21      3.23      2.24      2.18
         1.75      1.72      2.10      1.12
         8.11      6.18      5.65      4.11      2.76      1.90      1.91
         1.60      1.42      1.78      0.90
         CRED                -11.       250.
         CO        1.                  .5        -35.                .5
         12.9      19.4      14.2      11.6      11.6      11.6      11.6
         12.9      14.2      15.5      20.7
         EKMA      .17       10.       -10.      1.
         -1.       -1.       -.32      0.05      0.        0.009
         .6        .05
             BLANK
```

```
EXAMPLE 4 - EKMA OPTION - 1981 APPENDIX B PROCEDURES


PHOTOLYTIC RATE CONSTANTS CALCULATED FOR

         TEST CITY

LATITUDE      38.629
LONGITUDE     90.206
TIME ZONE     5.0
DATE          6     21    1986
TIME          800   TO    1800      LOCAL DAYLIGHT TIME


DILUTION DETERMINED FROM THE FOLLOWING
INVERSION HEIGHTS      INITIAL   250.      FINAL      1700.
TIMING                 START     800.      STOP       1500.


MIXING HEIGHTS (AT THE BEGINNING OF EACH HOUR)
TIME        800      900     1000     1100     1200     1300     1400     1500

HEIGHT      250.0    503.1    821.2   1119.5   1340.2   1496.2   1610.8   1700.0

REACTIVITY

EMISSIONS        ETH  FRACTION  .037   OLE  FRACTION  .035   ALD2 FRACTION  .052

EMISSIONS        FORM FRACTION  .021   TOL  FRACTION  .089   XYL  FRACTION  .117

EMISSIONS        PAR  FRACTION  .564   ISOP FRACTION  .000   NR   FRACTION  .085

SURFACE LAYER    ETH  FRACTION  .034   OLE  FRACTION  .020   ALD2 FRACTION  .037

SURFACE LAYER    FORM FRACTION  .070   TOL  FRACTION  .042   XYL  FRACTION  .026

SURFACE LAYER    PAR  FRACTION  .498   ISOP FRACTION  .000   NR   FRACTION  .273

ALOFT            ETH  FRACTION  .034   OLE  FRACTION  .020   ALD2 FRACTION  .037
ALOFT         FORM FRACTION  .070   TOL  FRACTION  .042   XYL  FRACTION  .026

ALOFT         PAR  FRACTION  .498   ISOP FRACTION  .000   NR   FRACTION  .273

NO2/NOX       .250
```

```
TRANSPORTED CONCENTRATIONS
SURFACE LAYER        OZONE     .060      HYDROCARBON   .080    NOX       .000 PPM
ALOFT                OZONE     .100      HYDROCARBON   .090    NOX       .009 PPM


CONTINUOUS EMISSIONS (EXPRESSED AS FRACTION OF THE INITIAL PRECURSORS)
SPECIES     HOUR         1      2      3      4      5      6      7      8      9     10
                        11

 VOC       FRACTION   .106   .086   .084   .058   .036   .025   .024   .020   .019   .024
                      .013

 NOX       FRACTION   .343   .262   .239   .174   .117   .080   .081   .068   .060   .075
                      .038

 CO        FRACTION   .045   .068   .050   .041   .041   .041   .041   .045   .050   .054
                      .072
```

```
EKMA CALCULATIONS ARE PERFORMED TO ESTIMATE

SITE-SPECIFIC VOC CONTROL REQUIREMENTS

BASE YEAR OZONE                                .170 PPM

BASE YEAR NMOC/NOX                           10.000

ANTICIPATED CHANGE IN NOX                   -10.000 PERCENT

FUTURE OZONE TRANSPORTED ALOFT                 .082 PPM

FUTURE NMOC TRANSPORTED ALOFT                  .050 PPMC

FUTURE NOX TRANSPORTED ALOFT                   .009 PPM

EMISSION CREDITS WILL BE ALLOWED FOR CO

ANTICIPATED CHANGE IN CO                    -35.000 PERCENT

FUTURE CO   TRANSPORTED ALOFT                  .500 PPM

MEDIAN CONTRIBUTION FACTOR FOR NMOC            .320

MEDIAN CONTRIBUTION FACTOR FOR NOX             .000

ADJUSTED NMOC/NOX                             6.800

FUTURE OZONE IN THE SURFACE LAYER              .054 PPM

FUTURE NMOC IN THE SURFACE LAYER               .048 PPMC

FUTURE NOX IN THE SURFACE LAYER                .000 PPM
```

```
                THE FOLLOWING SIMULATIONS WERE DONE.

    NMOC          NOX          RATIO          O3          TIME

  1.00000        .10000      10.00000       .23025      NOT MAX

   .73833        .07383      10.00000       .21136      NOT MAX

   .16532        .01653      10.00000       .15885      NOT MAX

   .28699        .02870      10.00000       .17195      NOT MAX

   .26890        .02689      10.00000       .17006      NOT MAX

   .18285        .02689       6.80000       .16866      NOT MAX

   .18430        .02710       6.80000       .16885      NOT MAX

   .19322        .02841       6.80000       .16995      NOT MAX

   .09661        .02557       3.77778       .13951      NOT MAX

   .08310        .02557       3.24958       .13816      NOT MAX

   .00000        .02557        .00000       .12903      NOT MAX


                COULD NOT FIND     .1200 OZONE IN   3 TRYS

                CHECK INPUT CONDITIONS OR GENERATE
                AN ISOPLETH DIAGRAM.
```

EXHIBIT 9

```
(   1)          1         2         3         4         5         6         7
(   2) 123456789012345678901234567890123456789012345678901234567890123456789012
(   3)
(   4) PLOT                           8.        5.6
(   5) TITL
(   6) EXAMPLE 5 - ISOPLETH OPTION USING MASS AND CREDIT OPTIONS
(   7) TRANS     .000      .080      0.       .05        0.        0.009
(   8) PLAC      38.629    90.206    5.0       1986.     6.0       21.
(   9) TEST CITY
(  10) DILU      250.      1700.
(  11) MASS      -11.      .6        0.05      250.
(  12) 9.42      7.68      7.54      5.21      3.23      2.24      2.18
(  13) 1.75      1.72      2.10      1.12
(  14) 8.11      6.18      5.65      4.11      2.76      1.90      1.91
(  15) 1.60      1.42      1.78      0.90
(  16) CRED                -11.       250.
(  17) CO        1.                  .5
(  18) 12.9      19.4      14.2      11.6      11.6      11.6      11.6
(  19) 12.9      14.2      15.5      20.7
(  20) SPEC      2.
(  21) O3        NO2
(  22) ISOP                          11.       1.                   2.
(  23) .06       .08       .10       .12       .14       .16        .18
(  24) .20       .22       .24       .26
(  25) .02       .03       .04       .05       .06       .07        .08
(  26) .09       .10       .12       .14
(  27)     BLANK
(  28)
(  29)          1         2         3         4         5         6         7
(  30) 123456789012345678901234567890123456789012345678901234567890123456789012
```

```
**************************************
*                                    *
*   OZONE ISOPLETH PLOTTING PACKAGE  *
*     WITH OPTIONAL MECHANISMS       *
*                                    *
*            O Z I P M               *
*                                    *
*          VERSION 4.00              *
*                                    *
*         DECEMBER, 1987             *
*                                    *
**************************************
```

EXHIBIT 10

```
THE INPUTS FOR THIS RUN ARE

          PLOT                           8.        5.6
          TITL
          EXAMPLE 5 - ISOPLETH OPTION USING MASS AND CREDIT OPTIONS
          TRANS     .000      .080      0.        .05       0.        0.009
          PLAC      38.629    90.206    5.0       1986.     6.0       21.
          TEST CITY
          DILU      250.      1700.
          MASS      -11.      .6        0.05      250.
          9.42      7.68      7.54      5.21      3.23      2.24      2.18
          1.75      1.72      2.10      1.12
          8.11      6.18      5.65      4.11      2.76      1.90      1.91
          1.60      1.42      1.78      0.90
          CRED                -11.       250.
          CO        1.                  .5
          12.9      19.4      14.2      11.6      11.6      11.6      11.6
          12.9      14.2      15.5      20.7
          SPEC      2.
          03        NO2
          ISOP                          11.       1.         2.
          .06       .08       .10       .12       .14       .16       .18
          .20       .22       .24       .26
          .02       .03       .04       .05       .06       .07       .08
          .09       .10       .12       .14
              BLANK
```

```
EXAMPLE 5 - ISOPLETH OPTION USING MASS AND CREDIT OPTIONS


PHOTOLYTIC RATE CONSTANTS CALCULATED FOR

         TEST CITY

LATITUDE      38.629
LONGITUDE     90.206
TIME ZONE     5.0
DATE          6     21    1986
TIME          800   TO    1800      LOCAL DAYLIGHT TIME

SOLAR NOON    1259

SUNRISE        542        SUNSET          2024


DILUTION DETERMINED FROM THE FOLLOWING
INVERSION HEIGHTS      INITIAL   250.      FINAL      1700.
TIMING                 START     800.      STOP       1500.


MIXING HEIGHTS (AT THE BEGINNING OF EACH HOUR)
TIME         800      900     1000     1100     1200     1300     1400     1500

HEIGHT      250.0    503.1    821.2   1119.5   1340.2   1496.2   1610.8   1700.0

REACTIVITY

EMISSIONS        ETH  FRACTION  .037   OLE  FRACTION  .035   ALD2 FRACTION  .052

EMISSIONS        FORM FRACTION  .021   TOL  FRACTION  .089   XYL  FRACTION  .117

EMISSIONS        PAR  FRACTION  .564   ISOP FRACTION  .000   NR   FRACTION  .085

ALOFT            ETH  FRACTION  .034   OLE  FRACTION  .020   ALD2 FRACTION  .037

ALOFT            FORM FRACTION  .070   TOL  FRACTION  .042   XYL  FRACTION  .026
ALOFT           PAR  FRACTION  .498   ISOP FRACTION  .000   NR   FRACTION  .273

NO2/NOX         .250
```

```
TRANSPORTED CONCENTRATIONS
ALOFT              OZONE     .080      HYDROCARBON   .050    NOX       .009 PPM


CONTINUOUS EMISSIONS (EXPRESSED AS FRACTION OF THE INITIAL PRECURSORS)
SPECIES     HOUR           1     2     3     4     5     6     7     8     9    10
                          11

  VOC      FRACTION     .106  .086  .084  .058  .036  .025  .024  .020  .019  .024
                        .013

  NOX      FRACTION     .343  .262  .239  .174  .117  .080  .081  .068  .060  .075
                        .038

  CO       FRACTION     .045  .068  .050  .041  .041  .041  .041  .045  .050  .054
                        .072
```

```
THE FOLLOWING SIMULATIONS WERE DONE.

NMOC     NOX        RATIO      O3          TIME      NO2         TIME

.00000   .00000      .00000  1.1630E-01    1800.   3.9657E-03    958.

.00000   .01400      .00000  1.2064E-01    1800.   9.6312E-03    913.

.00000   .02800      .00000  1.1701E-01    1800.   1.5481E-02    904.

.00000   .04200      .00000  9.5272E-02    1800.   2.0875E-02    903.

.00000   .05600      .00000  7.6894E-02    1800.   2.5778E-02    904.

.00000   .07000      .00000  6.6215E-02    1719.   3.0255E-02    906.

.00000   .08400      .00000  5.9402E-02    1631.   3.4350E-02    908.

.00000   .09800      .00000  5.4433E-02    1529.   3.8114E-02    909.

.00000   .11200      .00000  5.0773E-02    1512.   4.1603E-02    911.

.00000   .12600      .00000  4.7495E-02    1500.   4.4841E-02    912.

.00000   .14000      .00000  4.4663E-02    1452.   4.7854E-02    913.

.20000   .00000      .00000  1.2739E-01    1800.   3.4320E-03    940.

.20000   .01400    14.28571  1.3801E-01    1800.   9.5467E-03    906.

.20000   .02800     7.14286  1.4145E-01    1800.   1.5541E-02    901.

.20000   .04200     4.76190  1.3761E-01    1800.   2.1001E-02    902.

.20000   .05600     3.57143  1.1740E-01    1800.   2.5950E-02    903.

.20000   .07000     2.85714  9.3990E-02    1800.   3.0459E-02    905.

.20000   .08400     2.38095  7.9587E-02    1800.   3.4594E-02    907.

.20000   .09800     2.04082  6.9433E-02    1728.   3.8383E-02    909.
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.20000   .11200    1.78571  6.1949E-02   1654.  4.1892E-02   910.
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.40000   .01400   28.57143  1.4881E-01   1800.  9.4831E-03   858.
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.60000   .01400   42.85714  1.5427E-01   1800.  9.4234E-03   852.
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.60000   .04200   14.28571  1.7435E-01   1800.  2.1695E-02   857.
.60000   .05600   10.71429  1.7691E-01   1800.  2.6890E-02   900.
.60000   .07000    8.57143  1.7362E-01   1800.  3.1582E-02   902.
.60000   .08400    7.14286  1.5806E-01   1800.  3.5860E-02   905.
.60000   .09800    6.12245  1.3151E-01   1800.  3.9763E-02   907.
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.60000	.11200	5.35714	1.1094E-01	1800.	4.3349E-02	909.
.60000	.12600	4.76190	9.5755E-02	1800.	4.6679E-02	911.
.60000	.14000	4.28571	8.4007E-02	1800.	4.9767E-02	912.
.80000	.00000	.00000	1.2830E-01	1800.	2.7716E-03	921.
.80000	.01400	57.14286	1.5603E-01	1800.	9.3522E-03	848.
.80000	.02800	28.57143	1.7306E-01	1800.	1.6104E-02	851.
.80000	.04200	19.04762	1.8392E-01	1800.	2.2116E-02	854.
.80000	.05600	14.28571	1.9019E-01	1800.	2.7494E-02	857.
.80000	.07000	11.42857	1.9266E-01	1800.	3.2348E-02	900.
.80000	.08400	9.52381	1.8994E-01	1800.	3.6732E-02	903.
.80000	.09800	8.16326	1.7656E-01	1800.	4.0745E-02	906.
.80000	.11200	7.14286	1.5063E-01	1800.	4.4438E-02	908.
.80000	.12600	6.34921	1.2799E-01	1800.	4.7829E-02	910.
.80000	.14000	5.71429	1.1077E-01	1800.	5.0972E-02	912.
1.00000	.00000	.00000	1.2594E-01	1800.	2.6679E-03	918.
1.00000	.01400	71.42857	1.5559E-01	1800.	9.2745E-03	844.
1.00000	.02800	35.71428	1.7585E-01	1800.	1.6251E-02	848.
1.00000	.04200	23.80952	1.8980E-01	1800.	2.2496E-02	851.
1.00000	.05600	17.85714	1.9928E-01	1800.	2.8096E-02	855.
1.00000	.07000	14.28571	2.0528E-01	1800.	3.3133E-02	858.
1.00000	.08400	11.90476	2.0760E-01	1800.	3.7698E-02	901.
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1.00000   .11200     8.92857  1.9370E-01   1800.  4.5648E-02    907.
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1.00000   .14000     7.14286  1.4549E-01   1800.  5.2365E-02    911.
1.20000   .00000      .00000  1.2380E-01   1800.  2.5882E-03    916.
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1.20000   .07000    17.14286  2.1389E-01   1800.  3.3891E-02    856.
1.20000   .08400    14.28571  2.1934E-01   1800.  3.8653E-02    859.
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1.40000   .00000      .00000  1.2203E-01   1800.  2.5320E-03    915.
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1.40000   .07000    20.00000  2.1963E-01   1800.  3.4620E-02    854.
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1.40000   .09800    14.28571  2.3269E-01   1800.  4.4087E-02    900.
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1.60000   .01400  114.28570  1.5031E-01   1800.  9.0194E-03   838.
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1.60000   .09800   16.32653  2.4084E-01   1800.  4.5152E-02   858.
1.60000   .11200   14.28571  2.4568E-01   1800.  4.9453E-02   901.
1.60000   .12600   12.69841  2.4838E-01   1800.  5.3395E-02   904.
1.60000   .14000   11.42857  2.4748E-01   1800.  5.7022E-02   907.
1.80000   .00000     .00000  1.1898E-01   1800.  2.4324E-03   913.
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1.80000   .02800   64.28571  1.7305E-01   1800.  1.6477E-02   840.
1.80000   .04200   42.85714  1.9379E-01   1800.  2.3520E-02   843.
1.80000   .05600   32.14286  2.1114E-01   1800.  2.9969E-02   847.
1.80000   .07000   25.71429  2.2548E-01   1800.  3.5871E-02   850.
1.80000   .08400   21.42857  2.3693E-01   1800.  4.1242E-02   853.
1.80000   .09800   18.36735  2.4617E-01   1800.  4.6148E-02   856.
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1.80000   .14000   12.85714  2.6095E-01   1800.  5.8556E-02    905.

2.00000   .00000     .00000  1.1777E-01   1800.  2.3900E-03    912.

2.00000   .01400  142.85710  1.4678E-01   1800.  8.8423E-03    835.

2.00000   .02800   71.42857  1.7131E-01   1800.  1.6469E-02    839.

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2.00000   .05600   35.71428  2.1091E-01   1800.  3.0293E-02    845.

2.00000   .07000   28.57143  2.2641E-01   1800.  3.6382E-02    849.

2.00000   .08400   23.80952  2.3920E-01   1800.  4.1953E-02    852.

2.00000   .09800   20.40816  2.5002E-01   1800.  4.7079E-02    855.

2.00000   .11200   17.85714  2.5870E-01   1800.  5.1789E-02    858.

2.00000   .12600   15.87301  2.6553E-01   1800.  5.6089E-02    901.

2.00000   .14000   14.28571  2.7039E-01   1800.  6.0068E-02    903.
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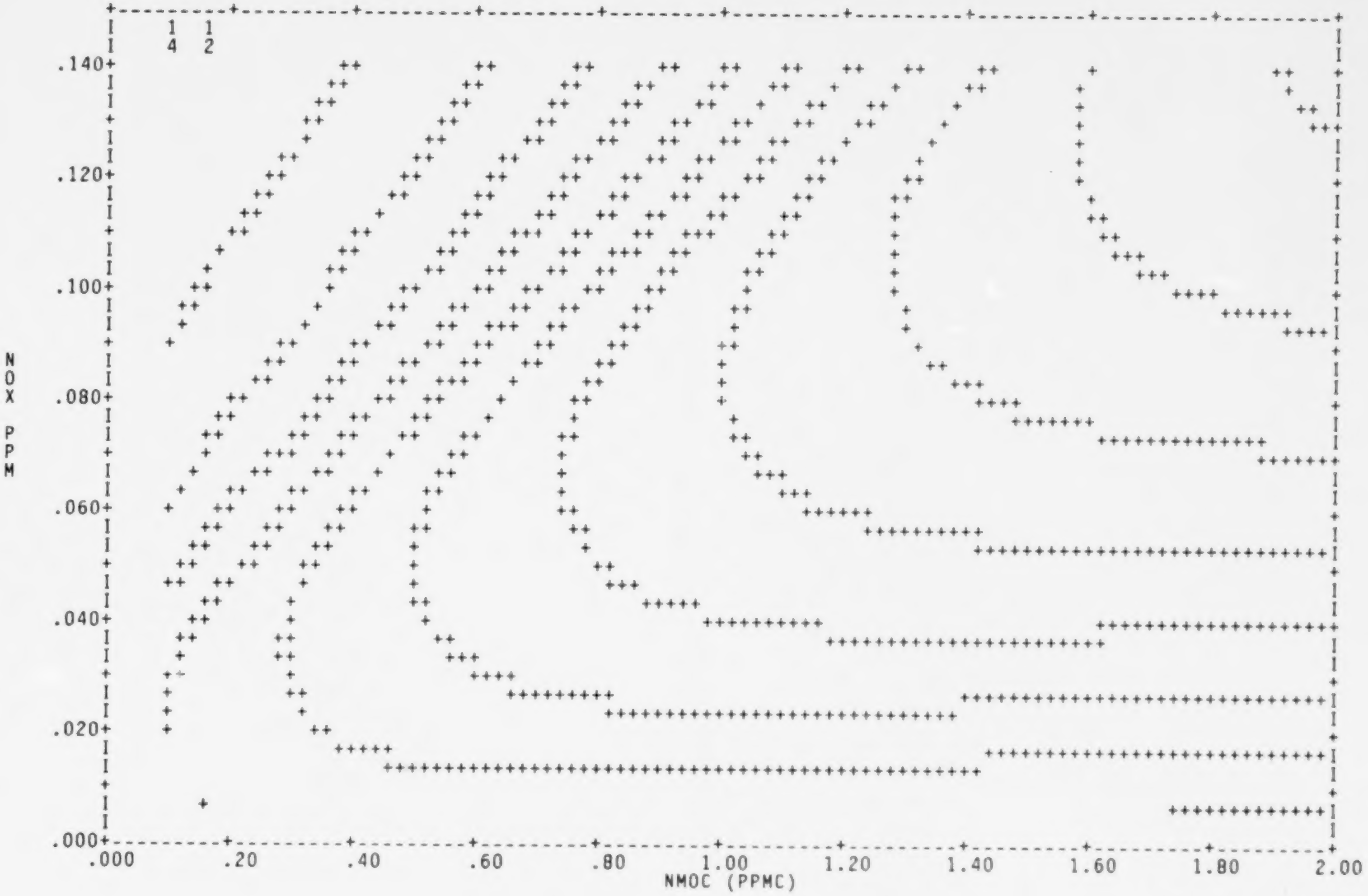
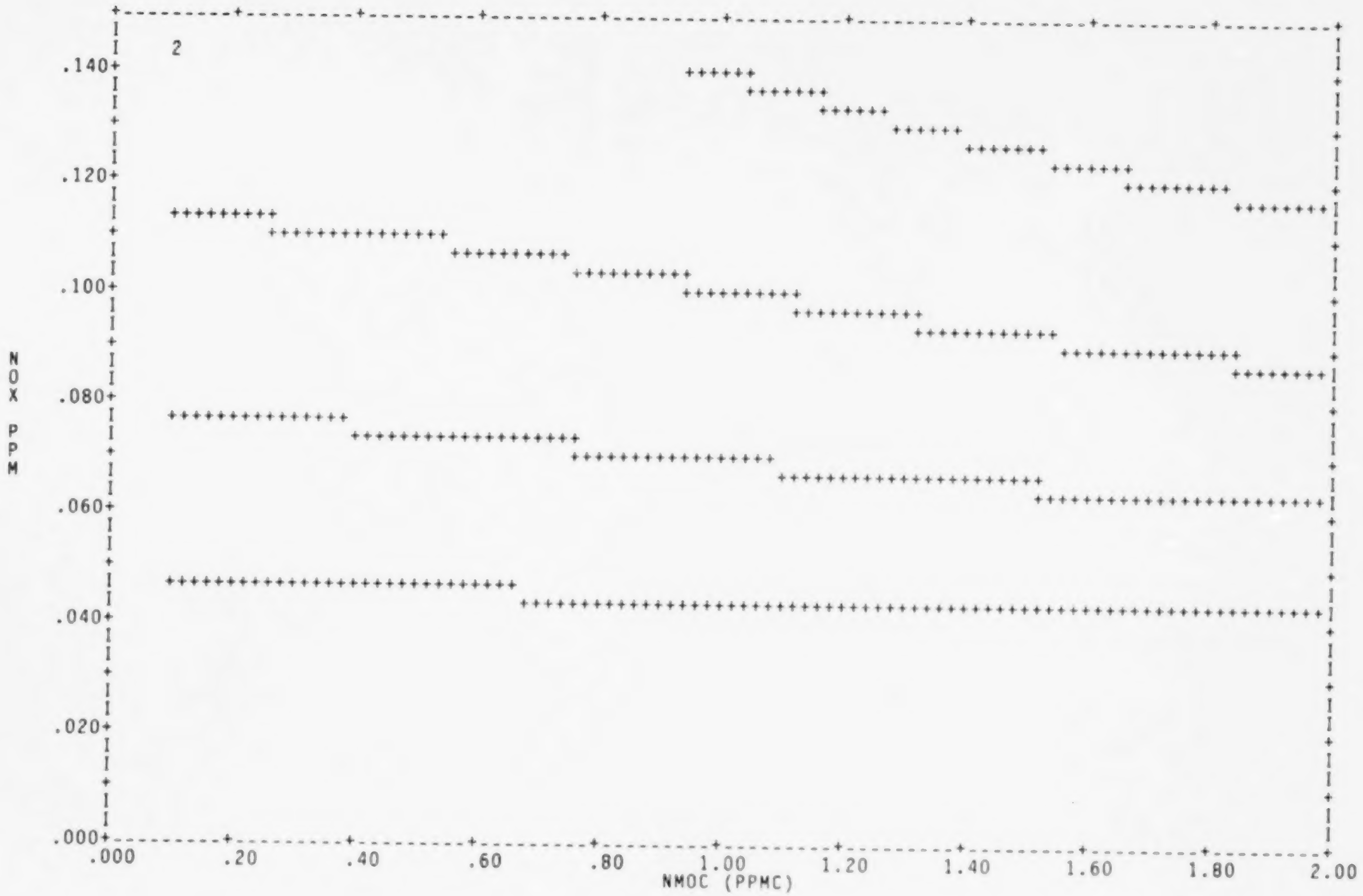


EXAMPLE 5 - ISOPLETH OPTION USING MASS AND CREDIT OPTIONS

THE O3 LINES ARE .06000 .08000 .10000 .12000 .14000 .16000 .18000 .20000 .22000 .24000
.26000



EXAMPLE 5 - ISOPLETH OPTION USING MASS AND CREDIT OPTIONS

THE NO2 LINES ARE .02000 .03000 .04000 .05000 .06000

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Appendix A

THE CARBON-BOND MECHANISM (CBM-IV)

TABLE A-1. The Carbon Bond Mechanism-IV.

Number	Reaction[1]	Reaction Rate Data		
		Pre-factor (ppm^{-n}min^{-1})	Temp. Factor exp((-E/R)/T)	Rate Constant @ 298K k_{298} (ppm^{-n}min^{-1})
1)	NO2 -hν--> NO + O			see notes
2)	O -----> O3	8.383 E+04	*EXP(1175/T)	4.323 E+06
3)	O3 + NO -----> NO2	2.643 E+03	*EXP(- 1370/T)	2.664 E+01
4)	O + NO2 -----> NO	1.375 E+04		1.375 E+04
5)	O + NO2 -----> NO3	2.303 E+02	*EXP(687/T)	2.309 E+03
6)	O + NO -----> NO2	3.233 E+02	*EXP(602/T)	2.438 E+03
7)	O3 + NO2 -----> NO3	1.760 E+02	*EXP(- 2450/T)	4.731 E-02
8)	O3 -hν--> O	5.300 E-02		5.300 E-02×k_1
9)	O3 -hν--> O1D			see notes
10)	O1D -----> O	1.147 E+05	*EXP(390/T)	4.246 E+05
11)	O1D + H2O -----> 2.00OH	3.260		3.260
12)	O3 + OH -----> HO2	2.344 E+03	*EXP(- 940/T)	1.000 E+02
13)	O3 + HO2 -----> OH	2.100 E+01	*EXP(- 580/T)	2.999
14)	NO3 -hν--> 0.89NO2 + 0.89O + 0.11NO	3.390 E+01		3.390 E+01×k_1
15)	NO3 + NO -----> 2.00NO2	1.909 E+04	*EXP(250/T)	4.416 E+04
16)	NO3 + NO2 -----> NO + NO2	3.660 E+01	*EXP(- 1230/T)	5.901 E-01
17)	NO3 + NO2 -----> N2O5	7.849 E+02	*EXP(256/T)	1.853 E+03
18)	N2O5 + H2O -----> 2.00HNO3	1.900 E-06		1.900 E-06
19)	N2O5 -----> NO3 + NO2	2.110 E+16	*EXP(-10897/T)	2.776
20)	NO + NO -----> 2.00NO2	2.600 E-05	*EXP(530/T)	1.539 E-04
21)	NO + NO2 + H2O -----> 2.00HONO	1.600 E-11		1.600 E-11
22)	OH + NO -----> HONO	6.554 E+02	*EXP(806/T)	9.799 E+03
23)	HONO -hν--> OH + NO	1.975 E-01		1.975 E-01×k_1
24)	OH + HONO -----> NO2	9.770 E+03		9.770 E+03
25)	HONO + HONO -----> NO + NO2	1.500 E-05		1.500 E-05
26)	OH + NO2 -----> HNO3	1.537 E+03	*EXP(713/T)	1.682 E+04
27)	OH + HNO3 -----> NO3	7.600	*EXP(1000/T)	2.179 E+02
28)	HO2 + NO -----> OH + NO2	5.482 E+03	*EXP(240/T)	1.227 E+04
29)	HO2 + NO2 -----> PNA	1.640 E+02	*EXP(749/T)	2.025 E+03
30)	PNA -----> HO2 + NO2	2.876 E+15	*EXP(-10121/T)	5.115
31)	OH + PNA -----> NO2	1.909 E+03	*EXP(380/T)	6.833 E+03
32)	HO2 + HO2 -----> H2O2	8.739 E+01	*EXP(1150/T)	4.144 E+03
33)	HO2 + HO2 + H2O -----> H2O2	7.690 E-10	*EXP(5800/T)	2.181 E-01
34)	H2O2 -hν--> 2.00OH	1.890 E-01		1.890 E-01×k_{39}
35)	OH + H2O2 -----> HO2	4.720 E+03	*EXP(- 187/T)	2.520 E+03
36)	OH + CO -----> HO2	3.220 E+02		3.220 E+02
37)	FORM + OH -----> HO2 + CO	1.500 E+04		1.500 E+04
38)	FORM -hν--> CO + 2.00HO2			see notes
39)	FORM -hν--> CO			see notes
40)	FORM + O -----> OH + HO2 + CO	4.302 E+04	*EXP(- 1550/T)	2.370 E+02
41)	FORM + NO3 -----> HNO3 + HO2 + CO	9.300 E-01		9.300 E-01
42)	ALD2 + O -----> C2O3 + OH	1.739 E+04	*EXP(- 986/T)	6.360 E+02
43)	ALD2 + OH -----> C2O3	1.037 E+04	*EXP(250/T)	2.400 E+04
44)	ALD2 + NO3 -----> C2O3 + HNO3	3.700		3.700
45)	ALD2 -hν--> FORM + XO2 + CO + 2.00HO2			see notes
46)	C2O3 + NO -----> NO2 + XO2 + FORM + HO2	7.915 E+03	*EXP(250/T)	1.831 E+04
47)	C2O3 + NO2 -----> PAN	1.180 E-04	*EXP(5500/T)	1.223 E+04
48)	PAN -----> C2O3 + NO2	5.616 E+18	*EXP(-14000/T)	2.220 E-02
49)	C2O3 + C2O3 -----> 2.00FORM + 2.00XO2 + 2.00HO2	3.700 E+03		3.700 E+03
50)	C2O3 + HO2 -----> 0.79FORM + 0.79XO2 + 0.79HO2 + 0.79OH	9.600 E+03		9.600 E+03
51)	OH -----> XO2 + FORM + HO2	6.521 E+03	*EXP(- 1710/T)	2.100 E+01

(Continued)

TABLE A-1. (Continued)

Number	Reaction[1]	Reaction Rate Data Pre-factor $(ppm^{-n}min^{-1})$	 Temp. Factor exp((-E/R)/T)	 Rate Constant @ 298K k_{298} $(ppm^{-n}min^{-1})$
52)	PAR + OH -----> 0.87XO2 + 0.13XO2N + 0.11HO2 + 0.11ALD2 + 0.76ROR - 0.11PAR	1.203 E+03		1.203 E+03
53)	ROR -----> 1.10ALD2 + 0.96XO2 + 0.94HO2 + 0.04XO2N + 0.02ROR - 2.10PAR	6.250 E+16	*EXP(- 8000/T)	1.371 E+05
54)	ROR -----> HO2	9.545 E+04		9.545 E+04
55)	ROR + NO2 ----->	2.200 E+04		2.200 E+04
56)	O + OLE -----> 0.63ALD2 + 0.38HO2 + 0.28XO2 + 0.30CO + 0.20FORM + 0.02XO2N + 0.22PAR + 0.20OH	1.756 E+04	*EXP(- 324/T)	5.920 E+03
57)	OH + OLE -----> FORM + ALD2 + XO2 + HO2 - PAR	7.740 E+03	*EXP(504/T)	4.200 E+04
58)	O3 + OLE -----> 0.50ALD2 + 0.74FORM + 0.33CO + 0.44HO2 + 0.22XO2 + 0.10OH - PAR	2.104 E+01	*EXP(- 2105/T)	1.800 E-02
59)	NO3 + OLE -----> 0.91XO2 + FORM + ALD2 + 0.09XO2N + NO2 - PAR	1.135 E+01		1.135 E+01
60)	O + ETH -----> FORM + 0.70XO2 + CO + 1.70HO2 + 0.30OH	1.540 E+04	*EXP(- 792/T)	1.080 E+03
61)	OH + ETH -----> XO2 + 1.56FORM + HO2 + 0.22ALD2	3.000 E+03	*EXP(411/T)	1.192 E+04
62)	O3 + ETH -----> FORM + 0.42CO + 0.12HO2	1.856 E+01	*EXP(- 2633/T)	2.700 E-03
63)	OH + TOL -----> 0.08XO2 + 0.[illegible]6CRES + 0.44HO2 + 0.56TO2	3.106 E+03	*EXP(322/T)	9.150 E+03
64)	TO2 + NO -----> 0.90NO2 + 0.90HO2 + 0.90OPEN	1.200 E+04		1.200 E+04
65)	TO2 -----> CRES + HO2	2.500 E+02		2.500 E+02
66)	OH + CRES -----> 0.40CRO + 0.60XO2 + 0.60HO2 + 0.30OPEN	6.100 E+04		6.100 E+04
67)	CRES + NO3 -----> CRO + HNO3	3.250 E+04		3.250 E+04
68)	CRO + NO2 ----->	2.000 E+04		2.000 E+04
69)	OPEN -hν--> C2O3 + HO2 + CO	8.400		8.400 *k_{38}
70)	OPEN + OH -----> XO2 + 2.00CO + 2.00HO2 + C2O3 + FORM	4.400 E+04		4.400 E+04
71)	OPEN + O3 -----> 0.03ALD2 + 0.62C2O3 + 0.70FORM + 0.03XO2 + 0.69CO + 0.08OH + 0.76HO2 + 0.20MGLY	8.030 E-02	*EXP(- 500/T)	1.500 E-02
72)	OH + XYL -----> 0.70HO2 + 0.50XO2 + 0.20CRES + 0.80MGLY + 1.10PAR + 0.30TO2	2.453 E+04	*EXP(116/T)	3.620 E+04
73)	OH + MGLY -----> XO2 + C2O3	2.600 E+04		2.600 E+04
74)	MGLY -hν--> C2O3 + HO2 + CO	8.960		8.960 *k_{38}
75)	O + ISOP -----> 0.60HO2 + 0.80ALD2 + 0.55OLE + 0.50XO2 + 0.50CO + 0.45ETH + 0.90PAR	2.700 E+04		2.700 E+04
76)	OH + ISOP -----> XO2 + FORM + 0.67HO2 + 0.40MGLY + 0.20C2O3 + 1.00ETH + 0.20ALD2 + 0.13XO2N	1.420 E+05		1.420 E+05
77)	O3 + ISOP -----> FORM + 0.40ALD2 + 0.55ETH + 0.20MGLY + 0.10PAR + 0.06CO + 0.44HO2 + 0.10OH	1.800 E-02		1.800 E-02
78)	NO3 + ISOP -----> XO2N	4.700 E+02		4.700 E+02
79)	XO2 + NO -----> NO2	1.200 E+04		1.200 E+04
80)	XO2 + XO2 ----->	2.550 E+01	*EXP(1300/T)	2.000 E+03
81)	XO2N + NO ----->	1.000 E+03		1.000 E+03
82)	NR -----> NR	1.000		1.000

(Continued)

TABLE A-1 (continued).

Notes:

1. Pressure dependent values for M, O_2 and CH_4 are included in the rate constant data (see text).

   $[M] = 1 \times 10^6$ ppm, $[O_2] = 2.095 \times 10^5$ ppm, and
   $[CH_4] = 1.85$ ppm.

   The symbols $h\nu$ in the reaction listing indicate photolysis reactions with rates dependent on zenith angle and solar irradiation. The basis for these rates is discussed in Section 4.

2. Chemical species in the CBM-IV are:

Species Name	Representation
Nitric Oxide	NO
Nitrogen Dioxide	NO2
Nitrogen Trioxide (nitrate radical)	NO3
Dinitrogen Pentoxide	N2O5
Nitrous Acid	HONO
Nitric Acid	HNO3
Peroxynitric acid (HO_2NO_2)	PNA
Oxygen Atom (singlet)	O1D
Oxygen Atom (triplet)	O
Hydroxyl Radical	OH
Water	H2O
Ozone	O3
Hydroperoxy Radical	HO2
Hydrogen Peroxide	H2O2
Carbon Monoxide	CO
Formaldehyde ($CH_2{=}O$)	FORM
High Molecular Weight Aldehydes (RCHO, R>H)	ALD2
Peroxyacyl Radical ($CH_3C(O)OO^{\cdot}$)	C2O3
Peroxyacyl Nitrate ($CH_3C(O)OONO_2$)	PAN
Paraffin Carbon Bond (C-C)	PAR
Secondary Organic Oxy Radical	ROR
Olefinic Carbon Bond (C=C)	OLE
Ethene ($CH_2{=}CH_2$)	ETH
Toluene ($C_6H_5{-}CH_3$)	TOL
Cresol and higher molecular weight Phenols	CRES

TALBE A-1 (concluded).

Species Name	Representation
Toluene-Hydroxyl Radical Adduct	TO2
Methylphenoxy Radical	CRO
High Molecular Weight Aromatic Oxidation Ring Fragment	OPEN
Xylene ($C_6H_4-(CH_3)_2$)	XYL
Methylglyoxal ($CH_3C(O)C(O)H$)	MGLY
Isoprene	ISOP
NO-to-NO_2 Operation	XO2
NO-to-Nitrate Operation	XO2N
Nonreactive Carbon	NR
TOTAL =	34

Appendix B

CBM-IV CARBON BOND GROUPS FOR ORGANIC SPECIES

TABLE B-1. Molecular weights of molecules (in alphabetical order).

SAROAD Code	Chemical Name	Molecular Weight
43814	1,1,1-TRICHLOROETHANE	133.42
43820	1,1,2-TRICHLOROETHANE	131.66
43813	1,1-DICHLOROETHANE	98.97
99013	1,1-DICHLOROETHENE	96.95
45225	1,2,3-TRIMETHYLBENZENE	120.19
45208	1,2,4-TRIMETHYLBENZENE	120.19
99016	1,2-DICHLOROPROPANE	112.99
45207	1,3,5-TRIMETHYLBENZENE	120.19
43218	1,3-BUTADIENE	54.09
46201	1,4-DIOXANE	88.12
98104	1-CHLOROBUTANE	92.57
43268	1-DECENE	140.27
98111	1-ETHOXY-2-PROPANOL	104.15
98113	1-HEPTANOL	116.21
98005	1-HEPTENE	98.18
43245	1-HEXENE	84.16
98037	1-METHYLCYCLOHEXANE	96.17
43267	1-NONENE	127.05
43224	1-PENTENE	70.13
43312	1-T-2-C-4-TM-CYCLOPENTANE	112.23
43269	1-UNDECENE	154.30
43296	2,2,3-TRIMETHYLPENTANE	114.23
43276	2,2,4-TRIMETHYLPENTANE	114.22
98033	2,2,5-TRIMETHYLHEXANE	128.26
43299	2,2,5-TRIMETHYLPENTANE	114.23
43291	2,2-DIMETHYLBUTANE	86.17
43280	2,3,3-TRIMETHYLPENTANE	114.22
43279	2,3,4-TRIMETHYLPENTANE	114.22
43234	2,3-DIMETHYL-1-BUTENE	84.16
98001	2,3-DIMETHYLBUTANE	86.17
43274	2,3-DIMETHYLPENTANE	100.20
98054	2,4,4-TRIMETHYL-1-PENTENE	112.22
98055	2,4,4-TRIMETHYL-2-PENTENE	112.22
43277	2,4-DIMETHYLHEXANE	114.22
43271	2,4-DIMETHYLPENTANE	100.20
43278	2,5-DIMETHYLHEXANE	114.22
98110	2-(2-BUTOXYETHOXY)-ETHANOL	162.18
43308	2-BUTYLETHANOL	118.17
98108	2-BUTYLTETRAHYDROFURAN	128.19
98051	2-CHLOROTOLUENE	126.59
43311	2-ETHOXYETHANOL	90.12

TABLE B-1. (Continued)

SAROAD Code	Chemical Name	Molecular Weight
43452	2-ETHOXYETHYL ACETATE	132.00
98002	2-ETHYL-1-BUTENE	84.16
98112	2-ETHYL-1-HEXANOL	130.23
43310	2-METHOXYETHANOL	76.09
43229	2-METHYL PENTANE	86.17
43225	2-METHYL-1-BUTENE	70.13
98040	2-METHYL-1-PENTENE	84.16
43228	2-METHYL-2-BUTENE	70.13
98004	2-METHYL-2-PENTENE	84.16
98076	2-METHYL-3-HEXANONE	114.19
43275	2-METHYLHEXANE	100.20
98032	3,5,5-TRIMETHYLHEXANE	128.26
98105	3-(CHLOROMETHYL)-HEPTANE	148.68
99021	3-CARENE	136.23
98041	3-HEPTENE	98.19
43230	3-METHYL PENTANE	86.17
43223	3-METHYL-1-BUTENE	70.13
43211	3-METHYL-1-PENTENE	84.16
43270	3-METHYL-T-2-PENTENE	84.16
43298	3-METHYLHEPTANE	114.23
43295	3-METHYLHEXANE	100.20
43293	4-METHYL-T-2-PENTENE	84.16
43297	4-METHYLHEPTANE	114.23
98042	4-NONENE	127.05
45221	A-METHYLSTYRENE	118.15
98025	A-PINENE	136.24
98097	A-TERPINEOL	154.24
43503	ACETALEHYDE	44.05
43404	ACETIC ACID	60.05
43551	ACETONE	58.08
43702	ACETONITRILE	41.05
43206	ACETYLENE	26.04
43505	ACROLEIN (ACRYLIC ALDHYDE)	56.06
43704	ACRYLONITRILE	53.06
98078	ALKENE KETONE	72.10
98085	ALKYL SUSTITUTED CYCLOHEXANE	132.21
99001	ALLYL CHLORIDE	76.53
98015	ANTHRACENE	178.22
98020	B-METHYLSTYRENE	118.15
98026	B-PINENE	136.24
45201	BENZENE	78.11

TABLE B-1. (Continued)

SAROAD Code	Chemical Name	Molecular Weight
45402	BENZOIC ACID	122.13
98024	BENZYL CHLORIDE	126.56
99017	BROMODICHLOROMETHANE	163.82
99019	BROMOFORM	252.77
98080	BUTANDIOL	90.12
43213	BUTENE	56.10
98074	BUTYL CELLOSOLVE	118.17
43510	BUTYRALDEHYDE	72.12
98035	C-2-HEXENE	84.16
43266	C-2-OCTENE	112.22
98003	C-3-HEXENE	84.16
43115	C-7 CYCLOPARAFFINS	98.19
43116	C-8 CYCLOPARAFFINS	112.23
43117	C-9 CYCLOPARAFFINS	126.26
98050	C10 AROMATICS	134.22
98039	C10 OLEFINS	140.27
98086	C2 ALKYL DECALIN	166.27
98084	C2 ALKYL INDAN	146.23
98064	C2 CYCLOHEXANE	112.22
43511	C3 ALDEHYDE	58.08
98068	C3 ALKYL CYCLOHEXANE	126.24
98065	C3 CYCLOHEXANE	126.24
98069	C4 ALKYL CYCLOHEXANE	140.27
98066	C4 CYCLOHEXANE	140.27
98070	C4 SUBSTITUTED CYCLOHEXANE	142.28
98073	C4 SUBSTITUTED CYCLOHEXANONE	154.26
43512	C5 ALDEHYDE	86.14
98067	C5 CYCLOHEXANE	154.30
98075	C5 ESTER	130.19
98071	C5 SUBSTITUTED CYCLOHEXANE	154.30
98095	C6 ALDEHYDE	100.17
43289	C6 OLEFINS	84.16
98072	C6 SUBSTITUTED CYCLOHEXANE	170.32
98093	C7 ESTER	158.24
43294	C7-OLEFINS	98.18
43513	C8 ALDEHYDE	128.21
43290	C8 OLEFINS	112.23
98049	C9 AROMATICS	120.20
98038	C9 OLEFINS	127.05
98096	CARBITOL	134.17

TABLE B-1. (Continued)

SAROAD Code	Chemical Name	Molecular Weight
98030	CARBON SULFIDE	76.14
43807	CARBON TETRABROMIDE	331.67
43804	CARBON TETRACHLORIDE	153.84
98031	CARBONYL SULFIDE	60.08
98087	CARVOMENTHOL	156.27
98088	CARVONE	150.22
43443	CELLOSOLVE ACETATE	132.00
99020	CHLORODIBROMOMETHANE	208.27
43825	CHLORODIFLUOROMETHANE (F-22)	86.47
43830	CHLOROFLUOROHYDROCARBONS	118.00
43803	CHLOROFORM	119.39
43827	CHLOROPENTAFLUOROETHANE(F-115)	154.47
99003	CHLOROPRENE	88.54
43826	CHLOROTRIFLUOROMETHANE (F-13)	104.46
43217	CIS-2-BUTENE	56.10
43227	CIS-2-PENTENE	70.13
98019	CRYOFLOURANE (F 114)	170.93
43248	CYCLOHEXANE	84.16
43264	CYCLOHEXANONE	98.15
43273	CYCLOHEXENE	82.14
43242	CYCLOPENTANE	70.14
43292	CYCLOPENTENE	68.11
43207	CYCLOPROPANE	42.08
98027	D-LIMONENE	136.24
43320	DIACETONE ALCOHOL	116.16
99015	DIBENZOFURAN	168.18
98107	DIBUTYL ETHER	130.23
43823	DICHLORODIFLOUROMETHANE (F-12)	120.91
43802	DICHLOROMETHANE	84.94
43828	DICHLOROTETRAFLUOROETHANE/114	170.92
98062	DIETHYLCYCLOHEXANE	140.27
98018	DIMETHYL ETHER	46.07
43450	DIMETHYL FORMAMIDE	73.09
98059	DIMETHYLCYCLOHEXANE	112.12
45103	DIMETHYLETHYLBENZENE	134.21
98091	DIMETHYLHEPTANE	128.26
98012	DIMETHYLNAPHTHALENE	156.22
98017	DM-2,3,DH-1H-INDENE	146.23
43287	DOCOSANE	310.59
43285	EICOSANE	282.54
99006	EPICHLOROHYDRIN	92.53

TABLE B-1. (Continued)

SAROAD Code	Chemical Name	Molecular Weight
43202	ETHANE	30.07
43433	ETHYL ACETATE	88.10
43438	ETHYL ACRYLATE	100.11
43302	ETHYL ALCOHOL	46.07
43812	ETHYL CHLORIDE	64.52
43351	ETHYL ETHER	74.12
98106	ETHYL ISOPROPYL ETHER	88.15
43219	ETHYLACETYLENE	54.09
43721	ETHYLAMINE	45.09
45203	ETHYLBENZENE	106.16
43288	ETHYLCYCLOHEXANE	112.23
98061	ETHYLCYCLOHEXANE	112.22
98057	ETHYLCYCLOPENTANE	98.19
43203	ETHYLENE	28.05
99014	ETHYLENE DIBROMIDE	187.88
43815	ETHYLENE DICHLORIDE	99.00
43370	ETHYLENE GLYCOL	62.07
43601	ETHYLENE OXIDE	44.05
98082	ETHYLHEPTENE	127.05
98011	ETHYLNAPHTHALENE	156.22
43502	FORMALDEHYDE	30.03
43368	GLYCOL	62.07
43367	GLYCOL ETHER	62.07
43286	HENEICOSANE	296.57
43282	HEPTADECANE	240.46
43232	HEPTANE	100.20
98077	HEPTANONE	114.18
99007	HEXACHLOROCYCLOPENTADIENE	272.77
43281	HEXADECANE	226.44
43231	HEXANE	86.17
43371	HEXYLENE GLYCOL	118.18
98044	INDAN	118.18
98048	INDENE	116.16
98115	ISOAMYL ISOBUTYRATE	158.24
43214	ISOBUTANE	58.12
43446	ISOBUTYL ACETATE	116.16
43306	ISOBUTYL ALCOHOL	74.12
43451	ISOBUTYL ISOBUTYRATE	144.21
98047	ISOBUTYLBENZENE	134.22
43215	ISOBUTYLENE	56.10
98036	ISOBUTYRALDEHYDE	72.11

TABLE B-1. (Continued)

SAROAD Code	Chemical Name	Molecular Weight
43120	ISOMERS OF BUTENE	56.10
45105	ISOMERS OF BUTYLBENZENE	134.21
43109	ISOMERS OF DECANE	142.28
45106	ISOMERS OF DIETHYLBENZENE	134.21
43112	ISOMERS OF DODECANE	170.33
45104	ISOMERS OF ETHYLTOLUENE	120.19
43106	ISOMERS OF HEPTANE	100.20
43105	ISOMERS OF HEXANE	86.17
43108	ISOMERS OF NONANE	128.25
43107	ISOMERS OF OCTANE	114.23
43114	ISOMERS OF PENTADECANE	212.41
43122	ISOMERS OF PENTANE	72.15
43121	ISOMERS OF PENTENE	70.13
43113	ISOMERS OF TETRADECANE	198.38
43111	ISOMERS OF TRIDECANE	184.36
43110	ISOMERS OF UNDECANE	156.30
45102	ISOMERS OF XYLENE	106.16
43243	ISOPRENE	68.13
43444	ISOPROPYL ACETATE	104.00
43304	ISOPROPYL ALCOHOL	60.09
98043	ISOPROPYLBENZENE (CUMENE)	120.20
98089	ISOPULEGONE	154.26
98056	ISOVALERALDEHYDE	86.14
43119	LACTOL SPIRITS	114.23
98022	M-CRESOL (3-M-BENZENOL)	110.16
98045	M-DIETHYLBENZENE	134.22
45212	M-ETHYLTOLUENE	120.19
45205	M-XYLENE	106.16
99008	MALEIC ANHYDRIDE	98.06
43201	METHANE	16.04
43432	METHYL ACETATE	74.08
43301	METHYL ALCOHOL	32.04
43445	METHYL AMYL ACETATE	140.00
43561	METHYL AMYL KETONE	114.19
43819	METHYL BROMIDE	94.95
43801	METHYL CHLORIDE	50.49
43552	METHYL ETHYL KETONE	72.10
98090	METHYL HEPTENE	112.22
43560	METHYL ISOBUTYL KETONE	100.16
98114	METHYL ISOBUTYRATE	102.13
43559	METHYL N-BUTYL KETONE	100.16

TABLE B-1. (Continued)

SAROAD Code	Chemical Name	Molecular Weight
43209	METHYLACETYLENE	40.06
98016	METHYLANTHRACENE	192.25
43261	METHYLCYCLOHEXANE	85.16
43262	METHYLCYCLOPENTANE	84.16
43272	METHYLCYCLOPENTENE	82.14
43805	METHYLENE BROMIDE	173.85
98010	METHYLNAPHTHALENE	142.19
45234	METHYLPROPYLBENZENE	134.21
43118	MINERAL SPIRITS	114.23
45801	MONOCHLOROBENZENE	112.56
43212	N-BUTANE	58.12
43435	N-BUTYL ACETATE	116.16
43305	N-BUTYL ALCOHOL	74.12
43238	N-DECANE	142.28
43255	N-DODECANE	170.33
43260	N-PENTADECANE	212.41
43220	N-PENTANE	72.15
98063	N-PENTYLCYCLOHEXANE	154.30
43303	N-PROPYL ALCOHOL	60.09
45209	N-PROPYLBENZENE	120.19
43259	N-TETRADECANE	198.38
43258	N-TRIDECANE	184.36
45101	NAPHTHA	114.23
98046	NAPHTHALENE	128.19
99009	NITROBENZENE	123.11
99010	NITROSOMORPHOLINE	116.11
43284	NONADECANE	268.51
43235	NONANE	128.25
98021	O-CRESOL (2-M-BENZENOL)	110.16
45211	O-ETHYLTOLUENE	120.19
45204	O-XYLENE	106.16
43283	OCTADECANE	254.49
43233	OCTANE	114.23
43265	OCTENE	112.21
98023	P-CRESOL (4-M-BENZENOL)	110.16
45807	P-DICHLOROBENZENE	147.01
45206	P-XYLENE	106.16
98094	PENTYL ALCOHOL	88.15
43817	PERCHLOROETHYLENE	165.85
45300	PHENOLS	94.11
43850	PHOSGENE (CCL2O)	98.92

TABLE B-1. (Concluded)

SAROAD Code	Chemical Name	Molecular Weight
98028	PHTHALIC ANAHYDRIDE	148.00
43208	PROPADIENE	40.06
43204	PROPANE	44.09
43504	PROPRIONALDEHYDE	58.08
43434	PROPYL ACETATE	102.13
45108	PROPYLBENZENE	120.19
98109	PROPYLCYCLOHEXANONE	140.23
43205	PROPYLENE	42.08
43369	PROPYLENE GLYCOL	76.09
43602	PROPYLENE OXIDE	58.08
98013	PROPYLNAPHTHALENE	170.25
45216	SEC-BUTYLBENZENE	134.21
45220	STYRENE	104.14
98116	SUBSTITUTED C7 ESTER (C12)	211.19
98117	SUBSTITUTED C9 ESTER (C12)	218.24
98034	T-2-HEXENE	84.16
98052	T-BUTYLBENZENE	134.22
43123	TERPENES	136.24
98079	TERPINENE	136.23
43309	TERT-BUTYL ALCOHOL	74.12
45215	TERT-BUTYLBENZENE	134.21
43390	TETRAHYDROFURAN	72.10
45232	TETRAMETHYLBENZENE	134.21
45202	TOLUENE	92.13
99018	TRANS-1,2-DICHLOROETHENE	96.95
43216	TRANS-2-BUTENE	56.10
43226	TRANS-2-PENTENE	70.13
45233	TRI/TETRAALKYL BENZENE	148.23
43824	TRICHLOROETHYLENE	131.40
43811	TRICHLOROFLOUROMETHANE	137.38
43821	TRICHLOROTRIFLOUROETHANE	187.38
43740	TRIMETHYL AMINE	59.11
45107	TRIMETHYLBENZENE	120.19
98060	TRIMETHYLCYCLOHEXANE	129.27
98058	TRIMETHYLCYCLOPENTANE	112.16
98083	TRIMETHYLDECENE	182.35
43822	TRIMETHYLFLUOROSILANE	92.00
98014	TRIMETHYLNAPHTHALENE	170.25
43241	UNDECANE	156.30
43860	VINYL CHLORIDE	62.50
45401	XYLENE BASE ACIDS	230.00

TABLE B-2. Species profiles by bond groups for CBM-IV.

SAROAD Code	Chemical Name	OLE	PAR	TOL	XYL	FORM	ALD2	ETH	ISOP	NR
43814	1,1,1-TRICHLOROETHANE	--	--	--	--	--	--	--	--	2
43820	1,1,2-TRICHLOROETHANE	--	--	--	--	--	--	--	--	2
43813	1,1-DICHLOROETHANE	--	--	--	--	--	--	--	--	2
99013	1,1-DICHLOROETHENE	--	--	--	--	--	--	1	--	--
45225	1,2,3-TRIMETHYLBENZENE	--	1	--	1	--	--	--	--	--
45208	1,2,4-TRIMETHYLBENZENE	--	1	--	1	--	--	--	--	--
99016	1,2-DICHLOROPROPANE	--	2	--	--	--	--	--	--	1
45207	1,3,5-TRIMETHYLBENZENE	--	1	--	1	--	--	--	--	--
43218	1,3-BUTADIENE	2	--	--	--	--	--	--	--	--
46201	1,4-DIOXANE	1	--	--	--	--	1	--	--	--
98104	1-CHLOROBUTANE	--	4	--	--	--	--	--	--	--
43268	1-DECENE	1	8	--	--	--	--	--	--	--
98111	1-ETHOXY-2-PROPANOL	--	3	--	--	--	1	--	--	--
98113	1-HEPTANOL	--	7	--	--	--	--	--	--	--
98005	1-HEPTENE	1	5	--	--	--	--	--	--	--
43245	1-HEXENE	1	4	--	--	--	--	--	--	--
98037	1-METHYLCYCLOHEXANE	--	7	--	--	--	--	--	--	--
43267	1-NONENE	1	7	--	--	--	--	--	--	--
43224	1-PENTENE	1	3	--	--	--	--	--	--	--
43312	1-T-2-C-4-TM-CYCLOPENTANE	--	8	--	--	--	--	--	--	--
43269	1-UNDECENE	1	9	--	--	--	--	--	--	--

TABLE B-2. (Continued)

SAROAD Code	Chemical Name	OLE	PAR	TOL	XYL	FORM	ALD2	ETH	ISOP	NR
43296	2,2,3-TRIMETHYLPENTANE	--	8	--	--	--	--	--	--	--
43276	2,2,4-TRIMETHYLPENTANE	--	8	--	--	--	--	--	--	--
98033	2,2,5-TRIMETHYLHEXANE	--	9	--	--	--	--	--	--	--
43299	2,2,5-TRIMETHYLPENTANE	--	8	--	--	--	--	--	--	--
43291	2,2-DIMETHYLBUTANE	--	6	--	--	--	--	--	--	--
43280	2,3,3-TRIMETHYLPENTANE	--	8	--	--	--	--	--	--	--
43279	2,3,4-TRIMETHYLPENTANE	--	8	--	--	--	--	--	--	--
43234	2,3-DIMETHYL-1-BUTENE	1	4	--	--	--	--	--	--	--
98001	2,3-DIMETHYLBUTANE	--	6	--	--	--	--	--	--	--
43274	2,3-DIMETHYLPENTANE	--	7	--	--	--	--	--	--	--
98054	2,4,4-TRIMETHYL-1-PENTENE	1	6	--	--	--	--	--	--	--
98055	2,4,4-TRIMETHYL-2-PENTENE	--	4	--	--	--	2	--	--	--
43277	2,4-DIMETHYLHEXANE	--	8	--	--	--	--	--	--	--
43271	2,4-DIMETHYLPENTANE	--	7	--	--	--	--	--	--	--
43278	2,5-DIMETHYLHEXANE	--	8	--	--	--	--	--	--	--
98110	2-(2-BUTOXYETHOXY)-ETHANOL	--	6	--	--	--	1	--	--	--
43308	2-BUTYLETHANOL	--	6	--	--	--	--	--	--	--
98108	2-BUTYLTETRAHYDROFURAN	--	6	--	--	--	1	--	--	--
98051	2-CHLOROTOLUENE	--	--	1	--	--	--	--	--	--
43311	2-ETHOXYETHANOL	--	2	--	--	--	1	--	--	--
43452	2-ETHOXYETHYL ACETATE	--	4	--	--	--	1	--	--	--
98002	2-ETHYL-1-BUTENE	--	5	--	--	1	--	--	--	--

TABLE B-2. (Continued)

SAROAD Code	Chemical Name	OLE	PAR	TOL	XYL	FORM	ALD2	ETH	ISOP	NR
98112	2-ETHYL-1-HEXANOL	--	8	--	--	--	--	--	--	--
43310	2-METHOXYETHANOL	--	1	--	--	--	1	--	--	--
43229	2-METHYL PENTANE	--	6	--	--	--	--	--	--	--
43225	2-METHYL-1-BUTENE	1	3	--	--	--	--	--	--	--
98040	2-METHYL-1-PENTENE	--	5	--	--	1	--	--	--	--
43228	2-METHYL-2-BUTENE	--	3	--	--	--	1	--	--	--
98004	2-METHYL-2-PENTENE	--	4	--	--	--	1	--	--	--
98076	2-METHYL-3-HEXANONE	--	7	--	--	--	--	--	--	--
43275	2-METHYLHEXANE	--	7	--	--	--	--	--	--	--
98032	3,5,5-TRIMETHYLHEXANE	--	9	--	--	--	--	--	--	--
98105	3-(CHLOROMETHYL)-HEPTANE	--	8	--	--	--	--	--	--	--
99021	3-CARENE	2	6	--	--	--	--	--	--	--
98041	3-HEPTENE	--	3	--	--	--	2	--	--	--
43230	3-METHYL PENTANE	--	6	--	--	--	--	--	--	--
43223	3-METHYL-1-BUTENE	1	3	--	--	--	--	--	--	--
43211	3-METHYL-1-PENTENE	1	4	--	--	--	--	--	--	--
43270	3-METHYL-T-2-PENTENE	--	4	--	--	--	1	--	--	--
43298	3-METHYLHEPTANE	--	8	--	--	--	--	--	--	--
43295	3-METHYLHEXANE	--	7	--	--	--	--	--	--	--
43293	4-METHYL-T-2-PENTENE	--	2	--	--	--	2	--	--	--
43297	4-METHYLHEPTANE	--	8	--	--	--	--	--	--	--
98042	4-NONENE	--	5	--	--	--	2	--	--	--

TABLE B-2. (Continued)

SAROAD Code	Chemical Name	OLE	PAR	TOL	XYL	FORM	ALD2	ETH	ISOP	NR
45221	A-METHYLSTYRENE	--	1	1	--	1	--	--	--	--
98025	A-PINENE	0.5	6	--	--	--	1.5	--	--	--
98097	A-TERPINEOL	1	6	--	--	--	1	--	--	--
43503	ACETALEHYDE	--	--	--	--	--	1	--	--	--
43404	ACETIC ACID	--	1	--	--	--	--	--	--	1
43551	ACETONE	--	3	--	--	--	--	--	--	--
43702	ACETONITRILE	--	1	--	--	--	--	--	--	1
43206	ACETYLENE	--	1	--	--	--	--	--	--	1
43505	ACROLEIN (ACRYLIC ALDHYDE)	1	--	--	--	1	--	--	--	--
43704	ACRYLONITRILE	1	1	--	--	--	--	--	--	--
98078	ALKENE KETONE	1	2	--	--	--	--	--	--	--
98085	ALKYL SUSTITUTED CYCLOHEXANE	--	9.5	--	--	--	--	--	--	--
99001	ALLYL CHLORIDE	1	1	--	--	--	--	--	--	--
98015	ANTHRACENE	--	6	--	1	--	--	--	--	--
98020	B-METHYLSTYRENE	--	--	1	--	--	1	--	--	--
98026	B-PINENE	1	8	--	--	--	--	--	--	--
45201	BENZENE	--	1	--	--	--	--	--	--	5
45402	BENZOIC ACID	--	--	1	--	--	--	--	--	--
98024	BENZYL CHLORIDE	--	--	1	--	--	--	--	--	--
99017	BROMODICHLOROMETHANE	--	--	--	--	--	--	--	--	1
99019	BROMOFORM	--	--	--	--	--	--	--	--	1
98080	BUTANDIOL	--	4	--	--	--	--	--	--	--

TABLE B-2. (Continued)

SAROAD Code	Chemical Name	OLE	PAR	TOL	XYL	FORM	ALD2	ETH	ISOP	NR
43213	BUTENE	1	2	--	--	--	--	--	--	--
98074	BUTYL CELLOSOLVE	--	4	--	--	--	1	--	--	--
43510	BUTYRALDEHYDE	--	2	--	--	--	1	--	--	--
98035	C-2-HEXENE	--	2	--	--	--	2	--	--	--
43266	C-2-OCTENE	--	4	--	--	--	2	--	--	--
98003	C-3-HEXENE	1	4	--	--	--	--	--	--	--
43115	C-7 CYCLOPARAFFINS	--	7	--	--	--	--	--	--	--
43116	C-8 CYCLOPARAFFINS	--	8	--	--	--	--	--	--	--
43117	C-9 CYCLOPARAFFINS	--	9	--	--	--	--	--	--	--
98050	C10 AROMATICS	--	3	1	--	--	--	--	--	--
98039	C10 OLEFINS	1	8	--	--	--	--	--	--	--
98086	C2 ALKYL DECALIN	--	12	--	--	--	--	--	--	--
98084	C2 ALKYL INDAN	--	4	1	--	--	--	--	--	--
98064	C2 CYCLOHEXANE	--	8	--	--	--	--	--	--	--
43511	C3 ALDEHYDE	--	1	--	--	--	1	--	--	--
98068	C3 ALKYL CYCLOHEXANE	--	9	--	--	--	--	--	--	--
98065	C3 CYCLOHEXANE	--	9	--	--	--	--	--	--	--
98069	C4 ALKYL CYCLOHEXANE	--	10	--	--	--	--	--	--	--
98066	C4 CYCLOHEXANE	--	10	--	--	--	--	--	--	--
98070	C4 SUBSTITUTED CYCLOHEXANE	--	10	--	--	--	--	--	--	--
98073	C4 SUBSTITUTED CYCLOHEXANONE	--	10	--	--	--	--	--	--	--
43512	C5 ALDEHYDE	--	3	--	--	--	1	--	--	--

TABLE B-2. (Continued)

SAROAD Code	Chemical Name	OLE	PAR	TOL	XYL	FORM	ALD2	ETH	ISOP	NR
98067	C5 CYCLOHEXANE	--	11	--	--	--	--	--	--	--
98075	C5 ESTER	--	7	--	--	--	--	--	--	--
98071	C5 SUBSTITUTED CYCLOHEXANE	--	11	--	--	--	--	--	--	--
98095	C6 ALDEHYDE	--	4	--	--	--	1	--	--	--
43289	C6 OLEFINS	1	4	--	--	--	--	--	--	--
98072	C6 SUBSTITUTED CYCLOHEXANE	--	12	--	--	--	--	--	--	--
98093	C7 ESTER	--	9	--	--	--	--	--	--	--
43294	C7-OLEFINS	1	5	--	--	--	--	--	--	--
43513	C8 ALDEHYDE	--	6	--	--	--	1	--	--	--
43290	C8 OLEFINS	1	6	--	--	--	--	--	--	--
98049	C9 AROMATICS	--	2	1	--	--	--	--	--	--
98038	C9 OLEFINS	1	7	--	--	--	--	--	--	--
98096	CARBITOL	--	2	--	--	--	2	--	--	--
98030	CARBON SULFIDE	--	1	--	--	--	--	--	--	--
43807	CARBON TETRABROMIDE	--	--	--	--	--	--	--	--	1
43804	CARBON TETRACHLORIDE	--	--	--	--	--	--	--	--	1
98031	CARBONYL SULFIDE	--	--	--	--	--	--	--	--	1
98087	CARVOMENTHOL	2	6	--	--	--	--	--	--	--
98088	CARVONE	2	6	--	--	--	--	--	--	--
43443	CELLOSOLVE ACETATE	--	3	--	--	--	1	--	--	1
99020	CHLORODIBROMOMETHANE	--	--	--	--	--	--	--	--	1
43825	CHLORODIFLUOROMETHANE (F-22)	--	--	--	--	--	--	--	--	1

TABLE B-2. (Continued)

SAROAD Code	Chemical Name	OLE	PAR	TOL	XYL	FORM	ALD2	ETH	ISOP	NR
43830	CHLOROFLUOROHYDROCARBONS	--	--	--	--	--	--	--	--	1
43803	CHLOROFORM	--	--	--	--	--	--	--	--	1
43827	CHLOROPENTAFLUOROETHANE(F-115)	--	--	--	--	--	--	--	--	2
99003	CHLOROPRENE	2	--	--	--	--	--	--	--	--
43826	CHLOROTRIFLUOROMETHANE (F-13)	--	--	--	--	--	--	--	--	1
43217	CIS-2-BUTENE	--	--	--	--	--	2	--	--	--
43227	CIS-2-PENTENE	--	1	--	--	--	2	--	--	--
98019	CRYOFLOURANE (F 114)	--	--	--	--	--	--	--	--	2
43248	CYCLOHEXANE	--	6	--	--	--	--	--	--	--
43264	CYCLOHEXANONE	--	6	--	--	--	--	--	--	--
43273	CYCLOHEXENE	1	4	--	--	--	--	--	--	--
43242	CYCLOPENTANE	--	5	--	--	--	--	--	--	--
43292	CYCLOPENTENE	1	3	--	--	--	--	--	--	--
43207	CYCLOPROPANE	--	3	--	--	--	--	--	--	--
98027	D-LIMONENE	1	4	--	--	--	2	--	--	--
43320	DIACETONE ALCOHOL	--	4	--	--	--	1	--	--	--
99015	DIBENZOFURAN	--	2	2	--	--	--	--	--	--
98107	DIBUTYL ETHER	--	6	--	--	--	1	--	--	--
43823	DICHLORODIFLOUROMETHANE (F-12)	--	--	--	--	--	--	--	--	1
43802	DICHLOROMETHANE	--	--	--	--	--	--	--	--	1
43828	DICHLOROTETRAFLUOROETHANE/114	--	--	--	--	--	--	--	--	2
98062	DIETHYLCYCLOHEXANE	--	10	--	--	--	--	--	--	--

TABLE B-2. (Continued)

SAROAD Code	Chemical Name	OLE	PAR	TOL	XYL	FORM	ALD2	ETH	ISOP	NR
98018	DIMETHYL ETHER	--	2	--	--	--	--	--	--	--
43450	DIMETHYL FORMAMIDE	--	--	--	--	--	--	--	--	3
98059	DIMETHYLCYCLOHEXANE	--	8	--	--	--	--	--	--	--
45103	DIMETHYLETHYLBENZENE	--	2	--	1	--	--	--	--	--
98091	DIMETHYLHEPTANE	--	9	--	--	--	--	--	--	--
98012	DIMETHYLNAPHTHALENE	--	4	--	1	--	--	--	--	--
98017	DM-2,3,DH-1H-INDENE	--	3	--	1	--	--	--	--	--
43287	DOCOSANE	--	22	--	--	--	--	--	--	--
43285	EICOSANE	--	20	--	--	--	--	--	--	--
99006	EPICHLOROHYDRIN	--	3	--	--	--	--	--	--	--
43202	ETHANE	--	0.4	--	--	--	--	--	--	1.6
43433	ETHYL ACETATE	--	3	--	--	--	--	--	--	1
43438	ETHYL ACRYLATE	--	1	--	--	--	2	--	--	--
43302	ETHYL ALCOHOL	--	2	--	--	--	--	--	--	--
43812	ETHYL CHLORIDE	--	--	--	--	--	--	--	--	2
43351	ETHYL ETHER	--	2	--	--	--	1	--	--	--
98106	ETHYL ISOPROPYL ETHER	--	3	--	--	--	1	--	--	--
43219	ETHYLACETYLENE	--	4	--	--	--	--	--	--	--
43721	ETHYLAMINE	--	1	--	--	--	--	--	--	1
45203	ETHYLBENZENE	--	1	1	--	--	--	--	--	--
43288	ETHYLCYCLOHEXANE	--	8	--	--	--	--	--	--	--
98061	ETHYLCYCLOHEXANE	--	8	--	--	--	--	--	--	--

TABLE B-2. (Continued)

SAROAD Code	Chemical Name	OLE	PAR	TOL	XYL	FORM	ALD2	ETH	ISOP	NR
98057	ETHYLCYCLOPENTANE	--	7	--	--	--	--	--	--	--
43203	ETHYLENE	--	--	--	--	--	--	1	--	--
99014	ETHYLENE DIBROMIDE	--	2	--	--	--	--	--	--	--
43815	ETHYLENE DICHLORIDE	--	--	--	--	--	--	1	--	--
43370	ETHYLENE GLYCOL	--	2	--	--	--	--	--	--	--
43601	ETHYLENE OXIDE	--	1	--	--	--	--	--	--	1
98082	ETHYLHEPTENE	1	7	--	--	--	--	--	--	--
98011	ETHYLNAPHTHALENE	--	5	1	--	--	--	--	--	--
43502	FORMALDEHYDE	--	--	--	--	1	--	--	--	--
43368	GLYCOL	--	2	--	--	--	--	--	--	--
43367	GLYCOL ETHER	--	2	--	--	--	--	--	--	--
43286	HENEICOSANE	--	21	--	--	--	--	--	--	--
43282	HEPTADECANE	--	17	--	--	--	--	--	--	--
43232	HEPTANE	--	7	--	--	--	--	--	--	--
98077	HEPTANONE	--	7	--	--	--	--	--	--	--
99007	HEXACHLOROCYCLOPENTADIENE	1	3	--	--	--	--	--	--	--
43281	HEXADECANE	--	16	--	--	--	--	--	--	--
43231	HEXANE	--	6	--	--	--	--	--	--	--
43371	HEXYLENE GLYCOL	--	6	--	--	--	--	--	--	--
98044	INDAN	--	2	1	--	--	--	--	--	--
98048	INDENE	1	--	1	--	--	--	--	--	--
98115	ISOAMYL ISOBUTYRATE	--	9	--	--	--	--	--	--	--

TABLE B-2. (Continued)

SAROAD Code	Chemical Name	OLE	PAR	TOL	XYL	FORM	ALD2	ETH	ISOP	NR
43214	ISOBUTANE	--	4	--	--	--	--	--	--	--
43446	ISOBUTYL ACETATE	--	6	--	--	--	--	--	--	--
43306	ISOBUTYL ALCOHOL	--	4	--	--	--	--	--	--	--
43451	ISOBUTYL ISOBUTYRATE	--	6	--	--	--	1	--	--	--
98047	ISOBUTYLBENZENE	--	3	1	--	--	--	--	--	--
43215	ISOBUTYLENE	--	1	--	--	1	1	--	--	--
98036	ISOBUTYRALDEHYDE	--	2	--	--	--	2	--	--	--
43120	ISOMERS OF BUTENE	--	--	--	--	--	2	--	--	--
45105	ISOMERS OF BUTYLBENZENE	--	3	1	--	--	--	--	--	--
43109	ISOMERS OF DECANE	--	10	--	--	--	--	--	--	--
45106	ISOMERS OF DIETHYLBENZENE	--	2	--	1	--	--	--	--	--
43112	ISOMERS OF DODECANE	--	12	--	--	--	--	--	--	--
45104	ISOMERS OF ETHYLTOLUENE	--	1	--	1	--	--	--	--	--
43106	ISOMERS OF HEPTANE	--	7	--	--	--	--	--	--	--
43105	ISOMERS OF HEXANE	--	6	--	--	--	--	--	--	--
43108	ISOMERS OF NONANE	--	9	--	--	--	--	--	--	--
43107	ISOMERS OF OCTANE	--	8	--	--	--	--	--	--	--
43114	ISOMERS OF PENTADECANE	--	15	--	--	--	--	--	--	--
43122	ISOMERS OF PENTANE	--	5	--	--	--	--	--	--	--
43121	ISOMERS OF PENTENE	--	1	--	--	--	2	--	--	--
43113	ISOMERS OF TETRADECANE	--	14	--	--	--	--	--	--	--
43111	ISOMERS OF TRIDECANE	--	13	--	--	--	--	--	--	--

TABLE B-2. (Continued)

SAROAD Code	Chemical Name	OLE	PAR	TOL	XYL	FORM	ALD2	ETH	ISOP	NR
43110	ISOMERS OF UNDECANE	--	11	--	--	--	--	--	--	--
45102	ISOMERS OF XYLENE	--	--	--	1	--	--	--	--	--
43243	ISOPRENE	2	1	--	--	--	--	--	--	--
43444	ISOPROPYL ACETATE	--	5	--	--	--	--	--	--	--
43304	ISOPROPYL ALCOHOL	--	3	--	--	--	--	--	--	--
98043	ISOPROPYLBENZENE (CUMENE)	--	2	1	--	--	--	--	--	--
98089	ISOPULEGONE	1	8	--	--	--	--	--	--	--
98056	ISOVALERALDEHYDE	--	3	--	--	--	1	--	--	--
43119	LACTOL SPIRITS	--	8	--	--	--	--	--	--	--
98022	M-CRESOL (3-M-BENZENOL)	--	--	1	--	--	--	--	--	--
98045	M-DIETHYLBENZENE	--	2	--	1	--	--	--	--	--
45212	M-ETHYLTOLUENE	--	1	--	1	--	--	--	--	--
45205	M-XYLENE	--	--	--	1	--	--	--	--	--
99008	MALEIC ANHYDRIDE	1	2	--	--	--	--	--	--	--
43201	METHANE	--	--	--	--	--	--	--	--	--
43432	METHYL ACETATE	--	--	--	--	--	--	--	--	3
43301	METHYL ALCOHOL	--	1	--	--	--	--	--	--	--
43445	METHYL AMYL ACETATE	--	8	--	--	--	--	--	--	--
43561	METHYL AMYL KETONE	--	7	--	--	--	--	--	--	--
43819	METHYL BROMIDE	--	--	--	--	--	--	--	--	1
43801	METHYL CHLORIDE	--	--	--	--	--	--	--	--	1
43552	METHYL ETHYL KETONE	--	4	--	--	--	--	--	--	--

TABLE B-2. (Continued)

SAROAD Code	Chemical Name	OLE	PAR	TOL	XYL	FORM	ALD2	ETH	ISOP	NR
98090	METHYL HEPTENE	1	6	--	--	--	--	--	--	--
43560	METHYL ISOBUTYL KETONE	--	6	--	--	--	--	--	--	--
98114	METHYL ISOBUTYRATE	--	5	--	--	--	--	--	--	--
43559	METHYL N-BUTYL KETONE	--	6	--	--	--	--	--	--	--
43209	METHYLACETYLENE	--	1.5	--	--	--	--	--	--	1.5
98016	METHYLANTHRACENE	--	9	--	1	--	--	--	--	--
43261	METHYLCYCLOHEXANE	--	7	--	--	--	--	--	--	--
43262	METHYLCYCLOPENTANE	--	6	--	--	--	--	--	--	--
43272	METHYLCYCLOPENTENE	1	4	--	--	--	--	--	--	--
43805	METHYLENE BROMIDE	--	--	--	--	--	--	--	--	1
98010	METHYLNAPHTHALENE	--	3	--	1	--	--	--	--	--
45234	METHYLPROPYLBENZENE	--	2	--	1	--	--	--	--	--
43118	MINERAL SPIRITS	--	6	--	--	--	1	--	--	--
45801	MONOCHLOROBENZENE	--	5	--	--	--	--	--	--	1
43212	N-BUTANE	--	4	--	--	--	--	--	--	--
43435	N-BUTYL ACETATE	--	5	--	--	--	--	--	--	1
43305	N-BUTYL ALCOHOL	--	2	--	--	--	1	--	--	--
43238	N-DECANE	--	10	--	--	--	--	--	--	--
43255	N-DODECANE	--	12	--	--	--	--	--	--	--
43260	N-PENTADECANE	--	15	--	--	--	--	--	--	--
43220	N-PENTANE	--	5	--	--	--	--	--	--	--
98063	N-PENTYLCYCLOHEXANE	--	11	--	--	--	--	--	--	--

TABLE B-2. (Continued)

SAROAD Code	Chemical Name	OLE	PAR	TOL	XYL	FORM	ALD2	ETH	ISOP	NR
43303	N-PROPYL ALCOHOL	--	3	--	--	--	--	--	--	--
45209	N-PROPYLBENZENE	--	2	1	--	--	--	--	--	--
43259	N-TETRADECANE	--	14	--	--	--	--	--	--	--
43258	N-TRIDECANE	--	13	--	--	--	--	--	--	--
45101	NAPHTHA	--	8	--	--	--	--	--	--	--
98046	NAPHTHALENE	--	2	--	1	--	--	--	--	--
99009	NITROBENZENE	--	1	--	--	--	--	--	--	5
99010	NITROSOMORPHOLINE	--	2	--	--	--	1	--	--	--
43284	NONADECANE	--	19	--	--	--	--	--	--	--
43235	NONANE	--	9	--	--	--	--	--	--	--
98021	O-CRESOL (2-M-BENZENOL)	--	--	1	--	--	--	--	--	--
45211	O-ETHYLTOLUENE	--	1	--	1	--	--	--	--	--
45204	O-XYLENE	--	--	--	1	--	--	--	--	--
43283	OCTADECANE	--	18	--	--	--	--	--	--	--
43233	OCTANE	--	8	--	--	--	--	--	--	--
43265	OCTENE	1	6	--	--	--	--	--	--	--
98023	P-CRESOL (4-M-BENZENOL)	--	--	1	--	--	--	--	--	--
45807	P-DICHLOROBENZENE	--	5	--	--	--	--	--	--	1
45206	P-XYLENE	--	--	--	1	--	--	--	--	--
98094	PENTYL ALCOHOL	--	5	--	--	--	--	--	--	--
43817	PERCHLOROETHYLENE	--	--	--	--	--	--	--	--	2
45300	PHENOLS	--	--	--	--	--	1	--	--	4

TABLE B-2. (Continued)

SAROAD Code	Chemical Name	OLE	PAR	TOL	XYL	FORM	ALD2	ETH	ISOP	NR
43850	PHOSGENE (CCL2O)	--	--	--	--	1	--	--	--	--
98028	PHTHALIC ANAHYDRIDE	--	--	--	1	--	--	--	--	2
43208	PROPADIENE	1.5	--	--	--	--	--	--	--	--
43204	PROPANE	--	1.5	--	--	--	--	--	--	1.5
43504	PROPRIONALDEHYDE	--	1	--	--	--	1	--	--	--
43434	PROPYL ACETATE	--	4	--	--	--	--	--	--	1
45108	PROPYLBENZENE	--	2	1	--	--	--	--	--	--
98109	PROPYLCYCLOHEXANONE	--	9	--	--	--	--	--	--	--
43205	PROPYLENE	1	1	--	--	--	--	--	--	--
43369	PROPYLENE GLYCOL	--	3	--	--	--	--	--	--	--
43602	PROPYLENE OXIDE	--	2	--	--	--	--	--	--	1
98013	PROPYLNAPHTHALENE	--	6	1	--	--	--	--	--	--
45216	SEC-BUTYLBENZENE	--	3	1	--	--	--	--	--	--
45220	STYRENE	--	--	1	--	1	--	--	--	--
98116	SUBSTITUTED C7 ESTER (C12)	--	10	--	--	--	--	--	--	2
98117	SUBSTITUTED C9 ESTER (C12)	--	10	--	--	--	--	--	--	2
98034	T-2-HEXENE	--	2	--	--	--	2	--	--	--
98052	T-BUTYLBENZENE	--	3	1	--	--	--	--	--	--
43123	TERPENES	1	8	--	--	--	--	--	--	--
98079	TERPINENE	2	6	--	--	--	--	--	--	--
43309	TERT-BUTYL ALCOHOL	--	--	--	--	--	--	--	--	4
45215	TERT-BUTYLBENZENE	--	1	1	--	--	--	--	--	3

TABLE B-2. (Concluded)

SAROAD Code	Chemical Name	OLE	PAR	TOL	XYL	FORM	ALD2	ETH	ISOP	NR
43390	TETRAHYDROFURAN	--	2	--	--	--	1	--	--	--
45232	TETRAMETHYLBENZENE	--	2	--	1	--	--	--	--	--
45202	TOLUENE	--	--	1	--	--	--	--	--	--
99018	TRANS-1,2-DICHLOROETHENE	--	--	--	--	--	--	1	--	--
43216	TRANS-2-BUTENE	--	--	--	--	--	2	--	--	--
43226	TRANS-2-PENTENE	--	1	--	--	--	2	--	--	--
45233	TRI/TETRAALKYL BENZENE	--	3	--	1	--	--	--	--	--
43824	TRICHLOROETHYLENE	--	--	--	--	--	--	1	--	--
43811	TRICHLOROFLOUROMETHANE	--	--	--	--	--	--	--	--	1
43821	TRICHLOROTRIFLOUROETHANE	--	--	--	--	--	--	--	--	2
43740	TRIMETHYL AMINE	--	3	--	--	--	--	--	--	--
45107	TRIMETHYLBENZENE	--	1	--	1	--	--	--	--	--
98060	TRIMETHYLCYCLOHEXANE	--	9	--	--	--	--	--	--	--
98058	TRIMETHYLCYCLOPENTANE	--	8	--	--	--	--	--	--	--
98083	TRIMETHYLDECENE	1	11	--	--	--	--	--	--	--
43822	TRIMETHYLFLUOROSILANE	--	--	--	--	--	--	--	--	3
98014	TRIMETHYLNAPHTHALENE	--	5	--	1	--	--	--	--	--
43241	UNDECANE	--	11	--	--	--	--	--	--	--
43860	VINYL CHLORIDE	--	--	--	--	--	--	1	--	--
45401	XYLENE BASE ACIDS	--	--	--	1	--	--	--	--	--